On High Pressure Real Gas Turbulent Mixing Jets

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ON HIGH PRESSURE REAL GAS TURBULENT MIXING JETS

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Abstract

A database of direct numerical simulation (DNS) of spatially evolving turbulent mixing slot jets of \( \text{C}_7\text{H}_{16}/\text{O}_2 \) and \( \text{C}_7\text{H}_{16}/\text{Air} \) is developed. The formulation includes the compressible form of the governing equations, a generalized multicomponent diffusion model with Soret and Dufour effects, a cubic real gas equation of state and realistic property models. Simulations are conducted over a wide range of initial pressures \((1\text{atm} < P_0 < 100\text{atm})\) and jet width based Reynolds numbers of 850 and 1300. High order explicit finite difference schemes in combination with low order boundary closures and Runge-Kutta time integration schemes are used to approximate the spatial and temporal derivatives. Non-reflecting inflow and outflow boundary conditions in combination with absorbing zones are applied for proper convection of flow structures and acoustic waves with minimal reflection of numerical waves. Low level disturbances are imposed on the laminar inflow near the nozzle to initiate instability for development of turbulence. The simulations are run until a statistically stationary state of the flow is achieved. The mean velocity, variance, centerline velocity excess decay, and downstream growth of normal Reynolds stresses are calculated and compared with various experimental results.

For subgrid analysis, a spatial filtering operation is applied to the DNS. The filtered mass density function (FMDF) of mixture fraction at various filter widths is obtained from the simulation at several spatial locations within the flow. The conditional scalar diffusion (CSD) term in the exact transport equation of FMDF is calculated from the DNS. A parametric study of variation of CSD with time, spatial location, Reynolds number, pressure and diffusion models is conducted. An \textit{a priori} analysis of Interaction by Exchange of Mean (IEM), Modified Curl (MC) and Mapping Closure (MAPPING) mixing models for CSD is conducted. Performance of mixing models at various pressures with the generalized and Fickian diffusion models, with real and ideal gas equations of state is evaluated. The significance of mixing frequency used in the models and the errors associated
with calculation of mixing frequency in simulations with the generalized diffusion model is studied. A parametric study of variation of the mixing frequency and its parameters with pressures, diffusion models and Reynolds number is performed. New model constants for mixing frequency applicable to the LES with generalized diffusion models at various pressures are proposed. Conditionally averaged mixing frequency for the IEM model is determined and compared with the conditionally averaged second invariant of the strain tensor to study the effects of flow physics (viscous dissipation) on the mixing time. Mean turbulent kinetic energy and mean dissipation rates are calculated from the DNS and their ratios are compared with mixing frequencies at various pressures. The model constants for various pressures are determined and an alternative expression for determination of mixing frequency in LES with generalized diffusion models is proposed.

The budget equation for the Reynolds stress tensor in the compressible RANS momentum equation is derived. The terms of the budget equation (convection, diffusion, pressure-strain, production, dissipation and compressibility) are calculated directly from the DNS at various pressures. The most significant terms in the budget that require modeling are determined to be diffusion and pressure-strain terms. Existing models for diffusion and pressure-strain terms are evaluated over a large range of pressures with the DNS data. At fixed Mach and Reynolds numbers, the models are determined to be dependent on the ambient pressure. New modeling constants for various models over a large range of pressures are proposed.
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...Dedicated to Amma, Appa, Bala and Preethi
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Chapter 1

Introduction

1.1 Problem Statement

Many modern day combustion devices such as rocket engines, diesel engines and gas turbines operate at pressures higher than atmospheric pressure. These devices encounter turbulent mixing and combustion at pressures of order \(10 \text{atm} \leq P \leq 100 \text{atm}\) [1]. Effective design and development of such devices require simulation tools. Reynolds Averaged Navier Stokes (RANS) and Large Eddy Simulation (LES) are two major approaches employed. Both approaches rely on accurate models to reproduce the effects of turbulent mixing and combustion. Turbulence is a multi-length scale phenomenon that occurs from length scales of order \(1m\) to \(10^3m\) (called Integral scales, for instance in atmospheric turbulence) to \(10^{-6}m\) to \(10^{-9}m\) (called Kolmogorov scales) before kinetic energy (KE) of the flow is dissipated as internal energy. In RANS, the time averaged equations of motion are solved to capture the mean flow properties and all the scales of turbulence are modeled. On the other hand, a spatial filter in the physical space is applied to the governing equations in LES to resolve all the large scale flow phenomena which are dependent on the initial and boundary conditions and only smaller scales of the flow are modeled. This is based on Kolmogorov’s (K41) theory [2, 3] that the small scale motions of turbulence are universal. Thus LES provides a better picture of the turbulent flow phenomena.

In LES, a number of modeling approaches have been proposed over the years to capture the essence of turbulent mixing and combustion. These models may be broadly classified as functional and structural models which typically aggregate the effects of small scale KE diffusion and dissi-
pation into a subgrid scale term. In other words, dissipation is assumed to take place at the scale determined by the filter size for LES, instead of the Kolmogorov scales. Most of these models reproduce the effects of turbulent mixing satisfactorily but result in large amount of errors in capturing the effects of chemical reaction since the chemical source term is highly non-linear.

A major relief in this area was obtained after introduction of the Probability Density Function (PDF) method by Pope [4], and the Filtered Density Function (FDF) and Filtered Mass Density Function (FMDF) approaches by Givi and his team [5, 6]. While PDF method is applied to RANS and in some cases to LES, the FDF and FMDF is applied largely to incompressible and compressible LES, respectively. In these methods, the complete statistical information of the flow is provided by a joint PDF or a filtered joint PDF (in case of FDF and FMDF) for velocity and / or scalars of the flow. A transport equation for this PDF is then derived. Solution of this transport equation provides all the moments of statistics of the flow. The main advantage of this approach is that the chemical source term is closed and does not require modeling. However, this transport equation results in some other terms that remain unclosed and require modeling. Two such terms that arise from this equation are subgrid scale (SGS) convection and conditional scalar diffusion (CSD), which physically represent the effects of molecular convection and molecular diffusion, respectively. The SGS convection is usually closed using a functional model like Smagorinsky or Eddy Viscosity model. The CSD is closed using models like Interaction by Exchange of Mean (IEM), Modified Curl (MC), Mapping Closure (MAPPING), and Euclidean Minimum Spanning Tree (EMST). While some models are more applicable than others in certain scenarios, each of the aforementioned models represent the molecular mixing phenomena fairly well. However, these models were predominantly developed using experimental data and direct numerical simulations (DNS) performed at 1 atm pressure with ideal gas assumptions. Thus these models have been observed to perform well at atmospheric pressures. The efficacy of these models at high pressures is yet unknown.

Although LES is a more accurate simulation technique to study turbulent flows, it requires considerable amount of computing resources and is still predominantly used as a research tool. RANS on the other hand is faster and requires the least amount of computing resources when compared to DNS and LES. As a result, RANS is the most preferred method of simulation in commercial tools. A wide range of modeling approaches are used in RANS. Some of the models are simple and easy to implement but lack accuracy while others are complex but produce more realistic results. The modeling approach depends on the application. One of the most accurate methods in RANS is the
Reynolds Stress Modeling (RSM) approach. In this a transport equation for the Reynolds stress tensor (source of turbulence in RANS) is derived and the terms of the equation are either directly resolved or modeled. Various models for the terms of the transport equation have been proposed for flows at atmospheric pressures. However, applicability of these models in high pressure flows have not been evaluated.

1.2 Research Objectives

The objectives of this research project are to:

- study the applicability of molecular mixing models used in LES, in flows at high pressures with multicomponent differential and cross diffusion effects and
- evaluate the applicability of diffusion and pressure-strain models used by RSM in RANS, in high pressure flows.

To achieve this a database of DNS of a spatially evolving turbulent slot jets at pressures of range 1 atm to 100 atm with real gas effects, realistic property models and a generalized diffusion model is developed. The spatially evolving turbulent jet enables measurement of FMDF and CSD from the flow at various spatial locations. The preliminary results indicate that the models have large dependency on mixing frequency which depends on the flow physics. Thus ambient pressure and diffusion models are determined to have significant effects on the mixing frequency. The spatially evolving flow also enables measurement of budget terms of the Reynolds stress transport equation. The terms of the equation and the terms of the model are computed from the DNS and compared over a large range of pressures. The models for diffusion and pressure-strain terms are also observed to vary significantly with pressure. In summary, this work investigates the effects of pressure on turbulent flow and some of the models used in turbulence.

This dissertation is organized into the following chapters. Chapter 1 outlines the general approaches taken by various authors to simulate spatially evolving turbulent flows. Chapter 2 presents the formulation for DNS conducted in this work and describes the computational framework, inflow conditions, initial conditions, boundary conditions and numerical approach used. Chapters (3,4) discuss the results of the topics discussed above.

In conclusion, this work will be the first to 1) perform direct numerical simulation of spatially
evolving slot jets at pressures $1\text{atm} \leq P_0 \leq 100\text{atm}$ with real gas properties, multicomponent cross-diffusion effects and real gas equation of state (EOS), 2) modify the Navier Stokes Characteristic Boundary Conditions (NSCBC) appropriately for proper convection of vortices in spatial flows at high pressures, 3) perform analysis of molecular mixing models used in LES, at high pressures with generalized and Fickian diffusion models and 4) perform analysis of RSM models used in RANS, at high pressures.

### 1.3 Need for Numerical Simulations of Spatially Evolving Flows

Turbulence is characterized by the appearance of complex structures in flows. The general theory for formation of complex flow structures is the cascading effect proposed by Richardson [7]. It suggests that the energy contained in the largest structures in a flow is dissipated as a result of breakup of vortices into smaller structures until the kinetic energy is dissipated by viscosity as internal energy. Thus, the length scales of turbulent flow structures in nature is seen to range from a few kilometers down to a few hundred nanometers. Experimental investigation of the phenomena requires a very large array of data acquisition equipment which is impractical and not economical for most types of complex flows in nature. Numerical simulations can largely mitigate this issue due to development of faster algorithms and large computing resources. Depending upon complexity of the flow and the required resolution and the type of simulation can be chosen.

In direct numerical simulations, the most commonly chosen flow configuration is temporally evolving flow which makes use of periodic boundary conditions in streamwise and spanwise directions. It represents evolution of flow in time at a fixed location in space. Such a simulation is easier to design and configure. However, the practical applications of temporally evolving flows are limited since they produce only one-point statistics in time. To gather multiple-point, multiple-time statistics a spatially evolving flow is required.

#### 1.3.1 General Issues with DNS of Spatially Evolving Flows

A spatially evolving flow requires physical boundary conditions that must be able to convect vortices, acoustic waves, entropy waves and numerical waves out of the computational domain while allowing pressure waves to propagate into the domain for realization of mean pressure [8, 9]. Such boundary conditions must be designed with care as issues may arise due to incompatibilities. This
may happen due to different boundary conditions at the interface of two or more boundaries or due to combinations of different boundary conditions at the same boundary. Instabilities may also arise as a result of different numerical schemes for the domain and boundaries. In addition, to resolve all the length and time scales of the turbulent flow, the grid resolution of computational domain must be very fine. Theoretically the number of grid points required to resolve a turbulent flow is set by the Reynolds number \( N_1 N_2 N_3 \sim Re^{2/3} \), where \( N_i (i = 1, 2, 3) \) indicates the number of grid points in a coordinate direction. This puts a limit on the maximum flow Reynolds number that can be simulated. This also means that size of the computational domain has to be very small with grid size of order \( \Delta x_i \approx \eta \), where \( \eta \) is the Kolmogorov scale.

Thus when the grid size is larger (due to fewer grid points or larger domain), the cascading effect is not observed at lower Reynolds numbers due to poor resolution of subgrid turbulent structures. However, with smaller grid size, the dispersion error generated increases by a large factor [10]. This can be mitigated by choosing a numerical scheme that is sufficiently dissipative. However, that introduces numerical dissipation which affects the solution. In temporal simulations, a highly non-dissipative scheme is generally preferred for internal and boundary closures, but such schemes cause incompatibility issues in spatial simulations. In DNS of high pressure flows, the strengths of acoustic waves and entropy waves increase with pressure. Furthermore to gather statistical data from turbulent flows, the simulation must be run until a statistically stationary state of the flow is reached. A turbulent flow becomes stationary when the statistics of the flow (mean, variance, joint probabilities) become invariant with time [11]. Thus the simulation must remain stable for long periods of time. The choice of numerical schemes, boundary conditions and inflow conditions for spatially evolving flows therefore become critical.

### 1.4 Literature Survey

Numerical simulation of spatially evolving flows is a challenge because of the aforementioned reasons, but it also provides a way to study various aspects of the flow and enables collection of numerous data that would otherwise be a tall task in an experiment. In the process of development of numerical simulations and models, it is important that the results from the simulations are validated using experimental data. This helps to deem the method fail-safe to replicate the results and be used to predict results when experiments cannot be performed. Thus development of
good numerical methods require thorough analysis of the physical phenomena being studied, survey of existing numerical tools, running multiple tests for various scenario with the available tools and careful documentation of the process. Some of the numerical tools may work in a number of different applications, while some others may work in very specific problems. Thus performing a survey of various attempts at tackling the problem is essential. In process of development of this DNS code, a number of test cases of spatially evolving flows were studied. These include pipe flows, mixing layers, round jets, square jets, rectangular jets, plane jets and slot jets. A survey of some of the approaches is presented in this section.

DNS of incompressible and low Mach number compressible turbulent jet flows were performed by Boersma [12], Danaila and Boersma [13], in which proper inflow conditions, boundary conditions and numerical methods applicable to simulation of spatially evolving jet flows were proposed. Boersma [14] further extended this to include the effects of chemical reaction at the low Mach number limit for compressible flows. A convection boundary condition was used in these studies which works well in the low Mach number limit. Modifications to convection boundary condition for non-cartesian coordinate system was proposed by Tam and Dong [15], Dong et al. [16]. However, this was applicable largely to one dimensional flows. Extension of Tam and Dong type boundary condition to three dimensional flows was proposed by Bogey and Bailey [17]. A combination of sponge layer and grid stretching method for outflow was also used in this study. Study on choice of appropriate reference values for variables in the sponge layer as described by Bogey and Bailey, for stable outflow of three dimensional compressible flows was performed by Uzun [18]. Lui [19] applied a combination of convection boundary condition and filtered stretched grid method for a stable outflow. Rembold [20] studied flow evolution of compressible rectangular jets by application of Dirichlet boundary condition and Thompson type boundary condition (characteristic wave based) [21] with sponge layers at the outflow. DNS of spatially evolving mixing layers using Dirichlet type boundary condition for inlet and Neumann type boundary condition for outflow was also performed by Ko et al. [22]. This work also included study of sensitivity of spatial flows to uncertain inflow conditions. Moore [23] compared the applicability of convection, Tam and Dong type, and Freund [24] boundary conditions with outflow filtering for highly compressible aeroacoustic flows. DNS of strongly buoyant compressible reacting flows using convection boundary condition was performed by Walchshofer et al. [25]. An empirical method to determine the appropriate time dependent convection velocity in convection boundary conditions was proposed by Pina et al. [26]. The idea
is to determine the convection velocity based on the intensity of outgoing waves obtained from the last few grid points of the domain. This method is reported to work better since it obviates the use of a constant convection velocity at the outflow which leads to stretching of flow structures and unphysical back flow many a times. DNS of incompressible spatially evolving flows were also performed by Aksellvol and Moin [27], Ruith et al. [28], Agarwal et al. [29], Gohil et al. [30], Trettel [31], Das and Garrick [32] which validate usage of convection type boundary condition for outflow of waves produced within computational domain.

Characteristic wave type boundary conditions introduced by Thompson was extended to include closures for viscous and diffusion terms by Poinsot and Lele [33]. This type of boundary condition is called Navier Stokes Characteristic Boundary Condition (NSCBC). It is applicable to subsonic compressible flows and has been widely used for simulation of spatially evolving compressible flows. Modifications to NSCBC for simulation of multiphase flows was proposed by Olsen [34]. Similar studies of multiphase flows with radiation and soot formation were performed by Wang [35] and Almeida and Jaberi [36]. Modification to NSCBC for entrainment of flow at the far fields, applicable for convection of large vortical structures in buoyant flows was proposed by Jiang and Luo [37, 38]. DNS of planar jet with NSCBC in combination with perfectly matched layers (PML) suggested by Hu et al. [39] was performed by Stanley and Sarkar [40]. The PML at the outflow ensures proper convection of acoustic waves outside the domain without any reflection. A similar approach using NSCBC and PML for outflow boundary was applied to simulate multiphase turbulent flow by Luo et al. [41]. The NSCBC was extended to include the real gas effects (real gas equation of state, properties of fluid applicable to high pressure flows) by Okong and Bellan [42]. A major drawback of NSCBC is that it assumes the flow at the outflow boundary to be locally one dimensional and inviscid. As a result, convection of three dimensional flow structures through boundaries can cause reflection of outgoing waves. Improvements to NSCBC by inclusion of transverse, viscous and chemical source terms for reacting flows were suggested by Sutherland and Kennedy [43]. Validation of this improved boundary condition for various types of spatially evolving flows by performed by Yoo and Im [44]. Lodato [45] proposed the extension of the improved boundary conditions (with transverse and viscous effects) to three dimensions by inclusion of treatments for the faces, edges and corners of the domain. This method is referred to as 3D-NSCBC. The 3D-NSCBC was further improved to include the real gas effects and validated for convection of vortices and strong acoustic waves by Coussement [46]. A comprehensive study of various boundary conditions and absorbing
layers for outflow applicable to spatial flows was performed by Colonius [8].

1.5 Boundary Conditions for Spatially Evolving Flows

In numerical simulations of partial differential equations (PDE) the oscillating solutions require a large distance from the source to dissipate naturally. One such case is that of the wave equation. This implies that a large computational domain (hence computational time and resources) would be required. However, for computational efficiency a truncated domain is desired. Truncation of computational grids many a times results in unphysical reflections. Specifying a Dirichlet boundary condition for a hyperbolic PDE results in reflection of the incident numerical wave. Hence for Navier Stokes equation, a hyperbolic form of boundary condition is desired. From the survey of DNS of spatial flows, the most effective boundary conditions are narrowed down to convection boundary condition and characteristic wave boundary condition in combination absorbing boundary conditions like sponge layers or perfectly matched layers. These boundary conditions were used at different stages of development stage of this DNS code. The following section will briefly explore these methods.

1.5.1 Convection Boundary Condition

This type of boundary condition was originally proposed by Sommerfeld [47] for the Helmholtz equation. It is also called radiation boundary condition. The idea was extended to numerical simulations of incompressible flows by Orlanski [48]. This method has been determined to be applicable to compressible flows at low Mach number limits as well. This boundary condition has a simple form,

\[ \frac{\partial \phi}{\partial t} + U_c \frac{\partial \phi}{\partial x} = 0, \]  

where \( U_c \) is the convection velocity that transports the variable \( \phi \) outside the boundary. For incompressible flows, the convection velocity at a boundary can usually be approximated to the mean velocity of the flow itself. However, for compressible flows, the convection velocity determination is not straightforward. Care must be taken to ensure that the convection velocity does not cause buildup of flow near boundaries or cause unphysical backflow. A value of convection velocity larger than the mean velocity (\( U_c > \overline{U} \), where \( \overline{U} \) is mean flow velocity) causes stretching of flow structures.
at the outflow. Sometimes in this case, the flow structures with large vorticity magnitudes spiral back into the domain. This leads to instability in the flow. A value of $U_c \leq \overline{U}$, results in build up of flow at the boundary and unphysical convection of waves. In some of the studies reported in the survey, a few techniques have been proposed to resolve this issue.

One of the methods is to add a small localized supersonic zone at exit of the computational domain (last few grid points). The convection velocity in this zone may be set to a supersonic magnitude. This causes all the properties to convect out of the domain without any reflection. Since high velocities cause stretching of flow near the exit, the convection velocity is steadily increased from a minimum value (typically mean velocity) at beginning of exit zone to supersonic value at the end of the exit zone. This may be expressed as,

$$U_{c,ss} = \left( \frac{x - x_{\text{start}}}{x_{\text{end}} - x_{\text{start}}} \right) U_{ss},$$

(1.2)

where $U_{ss}$ is the supersonic convection velocity, and $x_{\text{start}}, x_{\text{end}}$ are the start and end of the supersonic zone. This reduces the intensity of stretched flows near boundaries. Although circulation intensity of vortices can cause a slight backflow into the domain, the backflow usually exits the domain eventually. The exit zone is usually not considered for collection of flow statistics. Usage of supersonic exit zones are shown not to affect the flow upstream of the said zone. This modification in boundary condition works well for mixing flows but causes unphysical changes in pressure, density and temperatures in reacting flows.

### 1.5.2 Characteristic Boundary Condition

The idea of characteristic boundary condition is to transform the conserved form of compressible equations into an equation of form,

$$\frac{\partial U}{\partial t} + \lambda \frac{\partial U}{\partial x} = 0,$$

(1.3)

$\lambda$ in this equation is the characteristic convection velocity for the variable $U$ which can be determined for a given type of boundary condition. For a given boundary condition, the characteristic wave may enter or leave the computational domain and in the process dictate if information propagates into the domain or outside the domain. This is illustrated in Fig. 1.1. Unlike convection boundary
condition which prescribes same the convection velocity for all the properties, this type of boundary condition determines the appropriate convection velocities for each property. For a system with $M$ species and $N = M + 5$ variables, the characteristic waves may be derived as follows,

\[
U_{\text{conservative}} = U_{c,i} = [\rho, \rho u_1, \rho u_2, \rho u_3, \rho E, \rho Z_j],
\]

\[
U_{\text{primitive}} = U_{p,i} = [\rho, u_1, u_2, u_3, p, Z_j],
\]

\[
i = 1, \ldots N; j = 1, \ldots M.
\]

\[\text{\text{(1.4)}}\]

\[\rho \text{ in this equation represents the fluid density, } u_1, u_2, u_3 \text{ the velocities in each coordinate directions, } E \text{ the total energy, } Z_j \text{ the conserved scalars, and } p \text{ the total pressure. The choice of primitive variables is arbitrary but the conservative variables must be chosen carefully for a given problem.}\]

The conservation equations (Continuity, Navier Stokes, Energy, Species) may be written in general as,

\[
\frac{\partial U_{c,i}}{\partial t} + \frac{\partial F_k}{\partial x_k} + \frac{\partial D_k}{\partial x_k} = 0,
\]

\[\text{\text{(1.5)}}\]

where $F_k$ represents the flux terms and $D_k$ the diffusion terms of the equations. The quasi-linear form of the conservation equation is obtained by multiplying the above equation by the transformation matrix $P^{-1}$.

\[
P^{-1}[\frac{\partial U_{c,i}}{\partial t} + \frac{\partial F_k}{\partial x_k} + \frac{\partial D_k}{\partial x_k}] = \frac{\partial U_{p,i}}{\partial t} + f_k \frac{\partial U_{p,i}}{\partial x_k} + D_i = 0,
\]

\[\text{\text{(1.6)}}\]

where $P^{-1} = \frac{\partial U_{p,i}}{\partial U_{c,i}}$ and $f_k = \frac{\partial F_k}{\partial U_{c,i}}$. The characteristic form is then obtained by diagonalizing the Jacobian $f_k$, i.e. determining the matrix $S_k$ which satisfies,

\[
S_k^{-1}f_k S_k = \Lambda_k.
\]

\[\text{\text{(1.7)}}\]

The matrix $\Lambda_k$ is a diagonal matrix consisting of Eigenvalues of $f_k$. The characteristic waves are then defined as,

\[
L_i = \Lambda_i S_k^{-1}(\frac{\partial U_{p,i}}{\partial x_k}).
\]

\[\text{\text{(1.8)}}\]

Depending on the type of physical boundary condition required, the characteristic waves $L_i$ can be modified to either exit or enter the boundary by specifying the appropriate convection velocity. This boundary condition for primitive variables can be transformed back to boundary condition for
conservative variables through the transformation,

\[ Pd_i = PS_{k,i}L_i = PS_{k,i}A_i^k S_{k,i}^{-1} \frac{\partial U_p,i}{\partial x_k}, \]
\[ \frac{\partial U_{c,i}}{\partial t} + Pd_{i,1} + \frac{\partial F_l^i}{\partial x_l} + \frac{\partial D_l^i}{\partial x_l} = 0; l = 2, 3. \]  

This formulation is applicable to Euler equations in one dimension. This can be extended to Navier Stokes equations in three dimensions by deriving the transverse terms and either considering the fluid as inviscid or by treating the viscous terms in a similar fashion as presented above. This approach is more rigorous compared to treating convection boundary condition but is easy to implement. A detailed derivation of characteristic boundary conditions may be found in the works of Svendsen et al. [49], Thompson [21], and Lodato [45]. Modified form of characteristic boundary conditions are used in all the simulations presented in this work.

1.5.3 Absorbing Boundary Conditions

1.5.3.1 Sponge Layers

Sponge layers are artificial zones that in addition to outflow boundary conditions, may be added to a computational domain near the boundaries such that the intensity of any wave that enters this zone is reduced before it interacts with the outflow boundary. A few different types of sponge layers which stem from different concepts are presented in this section.

- Sponge layers in which the conservative variables of the flow are brought back to a set reference value was proposed by Wasistho et al. [50]. In this approach, the reference values of \( U_c = [\rho, \rho u_i, \rho E, \rho Y_j; i = 1, 2, 3, j = 1, \ldots M] \), are set to the free stream value and the conservative variables within the sponge zone are given as,

\[ U_c = U_{c,ref} + \sigma (U_c - U_{c,ref}), \]
\[ \sigma = \frac{x_i - x_{\text{start}}}{x_{\text{end}} - x_{\text{start}}}. \]  

\( x_{\text{start}}, x_{\text{end}} \) in this equation represent start and end of sponge zone and \( \sigma \) the function used to smoothly ramp the variables down to reference values within the sponge layer. This type of sponge layer is used in all of the simulations in this work. Some of the works cited in the literature [20, 51, 16, 19] use a different form of equation where flux of the governing equations
are reduced to a reference value instead of the conservative variables.

\[
\frac{\partial U_c}{\partial t} = RHS(U_c) - \sigma(U_c - U_{c_{\text{ref}}}).
\]  

(1.11)

- In another approach, a grid stretching algorithm and an internally biased scheme in combination with artificial viscosity or numerical filtering is used at the exit of the domain. The increased size of grids at the exit cause the turbulent structures to be less resolved as they exit the domain. An upwind or downwind biased scheme has the property of attenuating the disturbances produced from poorly resolved structures. In addition to this, an artificial viscosity may be prescribed in a small region near the exit such that these disturbances are reduced further. Colonius et al. [52] proposed usage of a low pass filter in the region where grid stretching is applied such that any high wave number disturbance reflected from the boundary would get weakened within this zone. This type of sponge layer is effective in mixing flows with low amplitude acoustic waves but requires a large number of grid points in the direction of flow.

1.5.3.2 Perfectly Matched Layers

Perfectly matched layer (PML) method for non-linear Euler and Navier Stokes equations was proposed by Hu et al. [39]. The idea of a PML is to exponentially absorb all the non-linear fluctuations produced in a flow within a small region near the boundaries such that the need for non-reflecting outflow boundary condition can be eliminated. Even if some waves reflect off of the boundary, they are attenuated within the PML zone. This is based on the PML method for absorption of electromagnetic waves proposed by Berenger [53]. The perfectly matched mean solutions for the linearized governing equations are prescribed within the PML. Although the absorbing equations for non-linear equations are not perfectly matched as their linearized counterpart, the numerical results are reported to be satisfactory. For non-linear equations, the solutions are split into time independent mean part and time dependent fluctuation part. The PML is designed to absorb the fluctuating part. When the time independent mean part of solution for a simulation is unknown on an apriori basis, a pseudo-mean flow is prescribed. For formulation of a PML, a proper space-time transformation is applied to the governing equations, then a complex change of variables is applied in frequency domain and absorbing boundary conditions are obtained by converting those equations.
back to time domain. A detailed derivation may be found in works of Hu et al. [39], Whitney et al. [54], Velu and Hoffman [55]. Although the PML method works very well in absorbing the fluctuations produced in wave equations, the method is complex. Care must be taken to when performing the complex change of variables and transforming from time domain to frequency domain and vice-versa. The choice of pseudo-mean flow is also essential and must be determined either by analytical methods or experimental results. Additionally, a number of equations must be solved simultaneously within the PML zone at every time step for the absorbing boundary to work. Thus it is not very practical to implement in computationally intensive codes.

1.6 Turbulence Modeling in LES

In LES, a spatial filter is applied to the governing equations in the physical space such that all the large flow structures that depend on the initial and boundary conditions (flow geometry) are resolved while the smaller subgrid scale (SGS) structures are modeled. The criteria for setting the filter width is not typically strict. It depends on the computational resources available. Depending on the filter width, the SGS terms may contain contribution from just the dissipative (Kolmogorov) scales or may contain elements of both inertial and dissipative scales. Flow at dissipative scales may be considered universal, but flow at inertial scales may not exhibit similar characteristics. Hence care must be taken to differentiate the two scales when modeling SGS terms. The general models for SGS may be classified as functional and structural models. In functional models the flow kinetic energy assumed is dissipate at the scale set by the filter width (with a SGS viscosity) instead of the dissipative scales. All the KE dissipation from filtered to Kolmogorov scales are lumped under a single sub-filtered dissipation term. Structural models on the other hand are more difficult to construct as they take into account the physics of formation of turbulent flow structures. Some of the modeling approaches use the idea of self-similarity in turbulent flows. Others divide the SGS stress term into SGS KE and SGS stress tensor and perform a weighted average. A review of some of the most widely used models including PDF based models is presented in Section (3.2).
1.7 Turbulence Modeling in RANS

In RANS, a Reynolds averaging operation is performed on variables of the flow. In this the flow variables are decomposed into time averaged (mean) and fluctuating components. This decomposition has certain properties which result in generation of mean flow equations from the governing equations. All the scales of motion of turbulent flows are modeled in RANS. Thus the resulting simulation is faster and generates the mean flow properties. However, accuracy of the solution is affected since all the effects of turbulence (at all scales) are lumped into a single source term (source of turbulence). Modeling in RANS refers to closure of this source term. The modeling approaches in RANS can be broadly classified into eddy viscosity models (linear and non-linear models) and Reynolds stress models. The former modeling approach uses constitutive relationships between the flow variables and the turbulent source term. These models attempt to reproduce the effects of turbulence using the flow variables that can be measured from the simulation itself. In the latter modeling approach, a transport equation is derived for the turbulence source term. The effects of turbulence is then obtained from solution of this transport equation. While this approach is more computationally intensive than eddy viscosity models, it is more accurate. A review of some of the modeling approaches used in RANS is presented in Section (4.1).

Figure 1.1: Characteristic Boundary Condition.
Chapter 2

DNS of a Transitional Slot Jet

2.1 Governing Equations

The DNS code in this work solves the compressible form of continuity, momentum, total energy and species mass fraction equations. This work uses both ideal gas and real gas equations of state, realistic property models, and multicomponent diffusion. The reader is referred to the work of Palle and Miller [56] for a detailed formulation.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} [\rho u_j] = 0, \tag{2.1}
\]

\[
\frac{\partial}{\partial t} (\rho u_i) + \frac{\partial}{\partial x_j} [\rho u_i u_j + P \delta_{ij} - \tau_{ij}] = 0, \tag{2.2}
\]

\[
\frac{\partial}{\partial t} (\rho e_t) + \frac{\partial}{\partial x_j} [\rho e_t u_j - u_i \tau_{ij} + Q_j + \sum_{\beta=1}^{N} H^3 J^3_j] = S_e, \tag{2.3}
\]

\[
\frac{\partial}{\partial t} (\rho Y^\beta) + \frac{\partial}{\partial x_j} [\rho Y^\beta u_j + J^\beta_j] = S_Y^\beta. \tag{2.4}
\]

In the above equations \(t\) represents time, \(x_j\) the spatial vector, \(\rho\) the density of mixture, \(u_j\) the mixture velocity vector, \(P\) the total pressure, \(\delta_{ij}\) the Kronecker delta tensor, \(\tau_{ij}\) the viscous stress tensor, \(e_t\) the total specific energy (internal energy plus kinetic energy), \(Q_j\) the heat flux vector,
\[ \sum_{\beta=1}^{N} \mathbf{H}^\beta, \mathbf{J}_j^\beta \] the enthalpy flux with \( N \) species, \( \mathbf{H}^\beta = \partial \mathbf{H} / \partial X^\beta \) the partial molar enthalpy of species \( \beta \), \( X^\beta \) the mole fraction of \( \beta \), \( \mathbf{J}_j^\beta \) the molar mass flux vector for species \( \beta \) (\( J_j^\beta = M_\beta \mathbf{J}_j^\beta \), where \( M_\beta \) represents the molecular weight of species \( \beta \)), and \( Y^\beta \) the mass fraction of species \( \beta \). The terms \( S_e \) and \( S^\beta_Y \) in the energy and species mass fraction equations represent the chemical reaction source terms. For mixing case the chemical source terms are considered to be zero (\( S_e = S^\beta_Y = 0 \)).

Real gas effects for high pressure simulations are included via cubic Peng Robinson equation of state. The Peng Robinson equation of state (PR EOS) is known to be computationally efficient and easy to implement [57]. It is expressed as,

\[
P = \frac{\mathcal{R} T}{\mathcal{v}} - \frac{A_m}{\mathcal{v}^2 + 2\pi B_m - B_m^2},
\]

where \( \mathcal{R} \) represents universal gas constant, \( T \) the temperature, \( \mathcal{v} \) the molar volume and \( A_m, B_m \) the mixture parameters defined for Peng Robinson equation of state [57, 58]. Ideal gas effects for simulations at atmospheric pressures is included via ideal gas equation of state [59],

\[
P = \rho \sum_{\beta} \frac{\mathcal{R}}{M_\beta} T.
\]

The heat flux and molar flux vectors with multicomponent differential and cross diffusion effects applicable to high pressure simulations are derived from Non-Equilibrium Thermodynamics (NEQT) and Keizer’s fluctuation theory. They may be expressed as,

\[
Q_j = - \left\{ \kappa + \sum_{\beta=1}^{N-1} \sum_{\gamma>\beta} N X_\beta X_\gamma \alpha_\beta^\gamma \alpha_\gamma^\beta \mathcal{R} \rho D_\beta^\gamma \left( \sum_{\beta_1=1}^{N} \frac{M_\beta}{M_m^2} X_\gamma \alpha_\beta^\gamma \rho D_\beta^\gamma \right) \alpha_\beta^\gamma \right\} \frac{\partial T}{\partial x_j}

- \sum_{\beta=1}^{N} \left\{ X_\beta \sum_{\gamma \neq \beta} \left[ \frac{M_\gamma}{M_m^2} X_\gamma \alpha_\beta^\gamma \rho D_\beta^\gamma \mathcal{V}_\beta \right] \frac{\partial P}{\partial x_j} \right\}

- \sum_{\eta=1}^{N-1} \sum_{\beta=1}^{N} \left\{ \mathcal{R} T \sum_{\gamma \neq \beta} \left[ \frac{M_\gamma}{M_m^2} X_\gamma \alpha_\beta^\gamma \rho D_\beta^\gamma \right] \alpha_\beta^\gamma \right\} \frac{\partial X_\beta}{\partial x_j},
\]
\[ J_j^\beta = -nD_m^{\beta\gamma} \sum_{\gamma \neq \beta}^N \left\{ X_\beta X_\gamma \frac{M_\gamma}{M_m} \alpha_{BK}^{\beta\gamma} \right\} \frac{\partial \ln T}{\partial x_j} \]

\[ - \sum_{\gamma \neq \beta}^N \frac{nD_m^{\beta\gamma}}{RT} \left\{ \frac{M_\beta M_\gamma}{M_m M_m} X_\beta X_\gamma \bar{v}_{\gamma} + \frac{M_\gamma M_\beta}{M_m M_m} X_\beta X_\gamma \bar{v}_{\beta} \right\} \frac{\partial P}{\partial x_j} \]

\[ - \sum_{\eta=1}^{N-1} \sum_{\gamma \neq \beta}^N \left\{ \left[ - \frac{M_\beta M_\gamma}{M_m M_m} X_\beta nD_m^{\beta\gamma} \alpha_{D}^{\gamma\eta} + \frac{M_\gamma M_\beta}{M_m M_m} X_\gamma nD_m^{\gamma\beta} \alpha_{D}^{\beta\eta} \right] \right\} \frac{\partial X_\eta}{\partial x_j}. \]

The general forms of the heat and molar flux vectors were first derived by Harstad and Bellan [60] for binary species mixing and extended to arbitrary number of species by Palle [57]. In the above equations, \( n \) represents the molar density (\( n = \rho/M_m \)), \( M_m = \sum_{\beta=1}^N X_\beta M_\beta \) the molecular weight of the mixture, \( \bar{v}_{\beta} \) the partial molar volume of species \( \beta \), \( D_m^{\beta\gamma} \) the mass diffusivities for diffusion of species \( \beta \) into species \( \gamma \), \( \kappa \) the mixture thermal conductivity, and \( \alpha_{BK}^{\beta\gamma}, \alpha_{D}^{\beta\eta} \) the thermal and mass diffusion factors.

### 2.2 Property Models

This DNS code uses realistic property models for mixture viscosity, thermal conductivity, heat capacities, mass diffusion coefficients and thermal diffusion coefficients to close Eqs.(2.1-2.8). The property models are based on principles of corresponding states or experimental data. Mixture viscosity and thermal conductivity is calculated by Lucas method [61] and the method of Steil and Thodos [61]. Heat capacities are calculated directly from the equation of state. The binary diffusion coefficients for low pressures are obtained by the method of Fuller et al. [61]. Coefficients for high pressures are obtained from the correlations of Takahashi [61]. Other significant differences between experimental data and property models were corrected by curve fitting models developed by Palle [57]. Binary thermal diffusion factors \( \alpha_{BK}^{\beta\gamma} \) for high pressures were obtained from curve fitting of experimental data by Vasudevan [58].

### 2.3 Flow Geometry

DNS of mixing and combustion at high Reynolds numbers are typically performed using a temporally evolving shear flow configuration with periodic boundary conditions in streamwise and
spanwise directions. This flow configuration is easier to implement but it generates only one point statistics in time. To generate multi-point flow statistics, a flow that evolves both in space and time is required. The flow configuration chosen for this study is that of a spatially evolving slot jet as presented in Fig. 2.1.

A cartesian coordinate system is used with \( x_1, x_2, x_3 \) describing the streamwise, cross-stream and spanwise directions, respectively. The overall domain length in each coordinate direction is chosen such that the flow is fully developed and the modifications to boundary conditions (sponge layer) have no effect on the flow where the statistics are gathered. The domain lengths in streamwise and cross-stream directions span from \( 0 < L_1 < 30D_{jet} \) and \( -10D_{jet} < L_2 < 10D_{jet} \), for \( Re_0 = 850 \) (nozzle jet width \( D_{jet} \), based Reynolds number) and from \( 0 < L_1 < 45D_{jet} \) and \( -15D_{jet} < L_2 < 15D_{jet} \), for a \( Re_0 = 1300 \). Length of domain in the spanwise direction is adjusted based on the number of grid points in \( x_1 \) and \( x_3 \) directions \( (L_3 = (N_3/1.5N_1)L_1) \). This is done to ensure same grid resolutions in cross-stream and spanwise directions. Domain length in spanwise direction ranges from \(-L_3/2 < L_3 < L_3/2\).

### 2.4 Numerical Approach

The governing equations are solved on equally spaced grids in all coordinate directions. A few cases use a mapping function in \( x_2 \) direction to compress the grids near the jet center line and stretch the grids near the boundaries. The mapping function used is similar to that of Foster [62]. However, the cases with grid compression were run only for testing purposes and statistics of the flow are not collected from them. For simulation of spatially evolving flows, compact finite difference schemes with spectral like resolutions are typically preferred. However, these schemes are not easy to parallelize. Thus to reduce the computational cost, eighth order explicit central finite difference schemes of Kennedy [63] are used for spatial discretization. This central finite difference scheme is closed at the boundary nodes using a scheme called 3-3-4-6-8 [64]. This scheme uses an internally biased third order stencil for nodes 1,2 and fourth and sixth order stencils at boundary nodes 3,4.
The boundary stencils are expressed as,

\[ f'_1 = \frac{1}{6\Delta x_1}(-11f_1 + 18f_2 - 9f_3 + 2f_4), \]
\[ f'_2 = \frac{1}{6\Delta x_1}(-2f_1 - 3f_2 + 6f_3 - f_4), \]
\[ f'_3 = \frac{2}{3\Delta x_1}(f_4 - f_2) - \frac{1}{12\Delta x_1}(f_5 - f_1), \]
\[ f'_4 = \frac{3}{4\Delta x_1}(f_5 - f_3) - \frac{3}{20\Delta x_1}(f_6 - f_2) + \frac{1}{60\Delta x_1}(f_7 - f_1). \]  

(2.9)

This low order scheme maintains numerical stability. It provides an overall fourth order spatial accuracy near the boundaries and has been proved to be stable. The second order derivatives in the viscous and diffusion terms are obtained by applying the first order derivative twice. The temporal derivatives for all the simulations are approximated by a fourth order Runge-Kutta scheme. Tenth order filtering for the spatial derivatives are applied at every Runge-Kutta stage to get rid of any spurious oscillations in the solutions [63]. CFL conditions for velocities, thermal and mass diffusivities are used for determine the minimum time step.

The number of grid points required for this study is based on the criteria \((N_1N_2N_3) \sim Re^{9/4}\) [65]. This criteria is obtained from dimensional analysis and is based on the fact that the ratio of Integral and Kolmogorov lengths scale as \(L/\eta \sim Re^{3/4}\). This provides a general guideline for the minimum number of grids required to resolve the smallest scales of the flow. Resolution of grids in every coordinate direction is set such that the statistics of the flow become independent of the resolution. Typical resolution at the jet centerline is of order \(\Delta x_i = 0.083D_{jet}\) in \(x_2, x_3\) directions and \(\Delta x_i = 0.1D_{jet}\) in \(x_1\) direction. The total number of grid points for this study range from 3.456 to 11.6 million.

This code is written in Fortran 77 and parallelized using MPI Fortran subroutines. The number of processors required for a simulation ranged from 256 to 864 CPUs. Table (2.1) provides details of the number of grid points and computing resource used for each test case.

### 2.5 Initial Conditions

The velocities of jet \((U_{jet} = 86.8m/s)\) and co-flow \((U_{co} = 17.4m/s)\) are chosen such that the transition to turbulence due to shear effects at the interface is maximized for the chosen forcing frequency. The convective Mach number represented by \(Ma_c\) is chosen to be 0.35 for all the simu-
lations in this study. The free stream densities and speeds of sound are calculated from the chosen equation of state. The initial flow Reynolds number \( Re_0 = \rho_{ref} U_{ref} D_{jet}/\mu_{ref} \) is calculated based on the reference velocity \( U_{ref} = U_{jet} - U_{co} \), reference density (average mixture density), reference viscosity (average mixture viscosity) and nozzle width of jet. In order to obtain a stationary flow, the simulation is performed for non-dimensional time \( t^* = t U_{ref}/D_{jet} \) of 200 to obtain converged statistics. Mean and variance of velocity in each coordinate direction is presented in Figs. 2.2-2.3. It is observed that the statistics of the flow become independent after \( t^* \geq 160 \). Mean and variance of velocity may be expressed as,

\[
\begin{align*}
\sigma^2 &= \langle (u'(t))^2 \rangle, \\
\langle u'(t) \rangle &= U(t) - \langle U \rangle, \\
\langle U \rangle &= \frac{1}{T} \int_0^T U(t) dt,
\end{align*}
\]  

(2.10)

where \( u'(t) \) represents the fluctuation of velocity about the mean and \( \langle U \rangle \) represents the time average of the flow at a given spatial location.

### 2.6 Boundary Conditions

In DNS of spatially evolving turbulent flows, formulation and implementation of proper boundary conditions is critical. As mentioned in Section (1.5), the outflow boundaries must be able to convect vortices, acoustic waves and entropy waves out of the computational domain while allowing pressure waves into the domain for realization of mean pressure.

In this work, the Navier Stokes Characteristic Boundary Condition (NSCBC) method proposed by Poinasot and Lele [33] is applied to all boundaries with appropriate modifications. The NSCBC method considers a boundary to be locally one-dimensional and inviscid (LODI). Characteristic convection velocities for each primitive variable in the governing equations is then derived. This characteristic velocity allows propagation of information outside the domain or vice-versa. This method works well in one or two dimensional flows away from edges or corners. In three dimensional flows the vortices, acoustic waves and entropy waves propagate outwards in a spherical fashion. When these waves reach the edges or corners of the domain, due to LODI nature of the boundary conditions they get reflected. The reflected waves travel upstream make and the numerical
scheme unstable. This causes solutions at the boundaries to crash. Three dimensional Navier Stokes Characteristic Boundary Conditions (3D NSCBC) proposed by Lodato et al. [66] avoids the LODI assumption by carefully treating every face, edge and corner of the domain while including effects of viscosity. However, these methods also increase the complexity of implementation of the boundary conditions and the required computation time.

This code makes use of the form of NSCBC proposed by O’kong and Bellan [42] along with a sponge layer in the $x_2$ direction. The formulation of NSCBC includes real gas effects. The sponge layer is similar to that of Wasistho et al. [67] where a given conservative variable is steadily brought back to its reference value. This reduces the intensity of outgoing wave through the characteristic boundary. It may be expressed as,

$$U_{c,i} = U_{c,ref} + f_1(U_{c,i} - U_{c,ref})$$

(2.11)

$$f_1 = \left[1 - C_1 f_2^2\right] \frac{1 - (1 - e^{c_2 f_2})}{1 - e^{c_2}}$$

(2.12)

$$f_2 = \frac{x_i - x_{\text{start}}}{x_{\text{end}} - x_{\text{start}}}$$

(2.13)

In the above equations, $U_{c,i}$ represents the conservative variables (density, momentum, energy, scalar), $U_{c,ref}$ the reference value for the corresponding conservative variable obtained from the free stream, $C_1, C_2$ the adjustable coefficients to change the strength of the sponge zone, and $x_{\text{start}}, x_{\text{end}}$ the start and end of sponge zone.

In $x_1$ direction, a subsonic non-reflecting outflow boundary condition is used where the convection velocities for all characteristic waves other than pressure is increased by a factor of local speed of sound ($\lambda_i + c$, $i=2,...,N$). This has an effect similar to the supersonic boundary condition discussed in Section (1.5) and allows realization of mean pressure within the domain. The amplitude of incoming wave is fixed at $C_K(p - p_\infty)$. The coefficient $C_K$ sets the intensity of incoming wave as proposed by Rudy and Strikwerda [68] and $p_\infty$ represents the ambient pressure inside the computational domain. Since this is applied only at the face of the outflow boundary, it does not cause stretching of the turbulent structure near boundaries or affect the incoming pressure wave. The flow region upstream of this boundary is observed to have no effects due to presence of this
boundary condition. The sponge zones used in $x_2$ direction prevent interaction of flow with corners of the computational domain at the outflow region. Periodic boundary condition is used in the $x_3$ direction.

A subsonic non-reflecting inflow boundary condition [33] is used at the inlet in $x_1$ direction. The inflow variables are subject to change with time due to upstream propagation of acoustic waves produced within the domain. This boundary condition allows the inflow velocities and temperature to be maintained at a target value.

2.7 Inflow Profile

To obtain a laboratory jet like flow profile at the inflow, the streamwise velocity in the shear layer on either side of the jet is given by a hyperbolic tangent function. It may be expressed as,

$$u(x_2) = \frac{U_{jet} + U_{co}}{2} - \frac{\Delta U_0}{2} \tanh\left(\frac{|x_2| - 0.5D_{jet}}{2\theta_0}\right),$$  \hspace{1cm} (2.14)

where $\theta_0 = 0.05D_{jet}$, is the shear layer momentum thickness, and $\Delta U_0 = U_{jet} - U_{co}$. This results in a symmetric top-hat velocity profile with smooth edges about the center-line. The cross-stream and spanwise velocities are specified as zero at the inflow. The mean pressure and temperature are initialized to be uniform throughout the domain. The mean profile for the species mass fractions is also given by a hyperbolic tangent function.

$$Y_{fuel} = 1 - \tanh\left(\frac{|x_2|}{2\theta_0}\right),$$  \hspace{1cm} (2.15)

$$Y_{ox} = 1 - Y_{fuel}.$$  

For multicomponent mixing like in the case of heptane-air, the initial mass fractions of oxygen and nitrogen are specified as $Y_{O_2} = 0.233Y_{ox}, Y_{N_2} = 0.767Y_{ox}$.

2.8 Turbulent Inflow Generation

In DNS of high Reynolds number spatially evolving flows, there is a natural transition of flow to turbulence at a distance away from the nozzle or inlet boundary. This is due to small perturbations which may arise from the numerical method or reflection of acoustic waves from the
boundaries. However, the distance at which flow transition takes place due to such perturbations is not predictable. In many cases flow transition may occur at a large distance from the nozzle. Thus, a larger computational domain might be required to observe turbulence in flow. In low Reynolds number flows, this natural transition to turbulence is further suppressed by the early onset of viscous dissipation. Thus, an artificial method of generating turbulent inflow is required.

A generally accepted forcing method for spatial flows is superimposition of artificial perturbations on the flow velocity at inflow [13, 30, 20, 40]. The perturbation term is usually a low amplitude sinusoidal term with a prescribed frequency. This is added to the streamwise velocity at every time step of the simulation \( A_f \sin(2\pi ft) \). However, there are no general guidelines for selection of forcing parameters. In many cases, the parameters are chosen by trial and error method. Furthermore, this method results in two dimensional forcing and transition to turbulence (observable cascading effect) occurs only at large Reynolds numbers. The velocity signal with this forcing method is not distributed over a large range of wave numbers and so the pseudo-turbulence gets dampened quickly. The velocity spectra is observed to be dominated by a single frequency (usually the forcing frequency). Other methods of generation of turbulent inflow include running an auxiliary simulation until development of turbulence, storing the cross-sectional slice of data and prescribing the stored flow properties at the inflow boundary of main simulation [69]. However, such a method requires lengthy runs of auxiliary simulations and proper rescaling of length and time scales of turbulent structures from auxiliary to main simulations. A digital filter based method for turbulence generation proposed by Klien [70] introduces a proper method of rescaling the length and time scales from auxiliary simulation while preserving the statistical moments of turbulence.

The forcing method used in this code combines the sinusoidal perturbation method with a circular spatial forcing term to induce spatio-temporal instability. The forcing term may be expressed as,

\[
\begin{align*}
    u_1(t) &= u_1(t) + A_f \sin(2\pi ft) \theta, \\
    \theta &= \tan^{-1}(\frac{x_3}{x_2}),
\end{align*}
\]

where \( A \) represents the amplitude of forcing signal which is chosen to be a value between 0.001-0.002 (larger amplitudes cause production of stronger numerical waves that corrupt the flow, while perturbations with smaller amplitudes get dampened quickly) and \( f \) represents the most unstable
frequency which determines the distance away from inlet at which flow transition takes place. Based on a number of simulations performed, a value of $f$ between 0.25-0.4 is chosen such that the distance of flow transition is less than $x_1 = 10D_{jet}$ from nozzle. However, these perturbation frequencies work only for velocities ($U_{jet} = 86.8$m/s, $U_{co} = 17.4$m/s). For flows with different velocities, the most unstable frequency may be determined from linear stability analysis [71]. The circular spatial forcing term $\theta = \theta(x_2, x_3)$ induces three dimensional spatial instability. Instability in spatial flows is induced when the wave number is complex and wave frequency is real ($u'(y, t) = u(y) \exp(i(kx - \omega t))$, with $k$ - complex, $\omega$ - real). Since the boundaries in spanwise directions are periodic, a forcing method without $\theta$ does not induce cascading.

A comparison of flow evolution with different forcing frequencies and effect of the spatial forcing term ($\theta$) is presented in Fig. 2.4. It is observed that without $\theta$, the flow evolution is largely two dimensional. A value of frequency $f < 0.2$, causes production of a strong acoustic waves very close to the inflow boundary. This causes large reflections of waves at the inflow boundary and failure of the boundary condition. A frequency of $f > 0.4$, further increases the distance of flow transition from the inflow boundary. The Fast Fourier transform of the velocity signal obtained from this flow is initially observed to be dominated largely by the forcing frequency. However, after application of a high pass filter other frequencies contained within the flow become evident as observed in Fig. 2.5.

### 2.9 Results

#### 2.9.1 Structural Evolution of Jet

The simulation is started with a laminar flow profile throughout the domain and the inflow perturbation is then turned on. The transition process may be visualized with instantaneous two dimensional contour plots of density (at $P_0 = 1atm$, 100atm and $Re_0 = 850, 1300$) in Figs. 2.6-2.9 and mixture fraction in Fig. 2.10. It is observed that in the region $x_1 < 10D_{jet}$ in flow at $Re_0 = 850$ and $x_1 < 14D_{jet}$ in flow at $Re_0 = 1300$, the flow is laminar. Roll up of vortex rings due to Kelvin Helmholtz instability [72] is observed in the region $10D_{jet} < x_1 < 15D_{jet}$ at $Re_0 = 850$ and $14D_{jet} < x_1 < 18D_{jet}$ at $Re_0 = 1300$. These vortices represent emergence of varicose modes from the sinusoidal perturbations. These vortex rings move downstream and begin to pair. This corresponds to natural subharmonic perturbations generated after formation of primary vortices. Further downstream, these structures breakup and indicate the cascading effect. Around $x_1 > L_x/2$, ...
the jet potential core ends and the flow becomes fully turbulent. At both initial pressures, the flow at $Re_0 = 850$ is observed to have smaller and uniform jet spread angle. At $P_0 = 1\text{ atm}$ and $Re_0 = 1300$ the jet spread angle is observed to be slightly non-uniform, but at $P_0 = 100\text{ atm}$, the spread angle is observed to be transient and highly non-uniform. This is due to the presence of strong acoustic waves at large pressures and higher Reynolds numbers which cause large instabilities in the flow.

2.9.2 Mean Velocity of Flow

Time averaged statistics of flow variables are calculated and compared against experimental results to validate the DNS data. Although the flow profile in this work is a slot jet, the flow evolution is structurally similar to a plane jet. Thus the flow evolution is validated against experimental results from both slot jets and plane jets. Mean velocity excess in jets describe the spatial evolution of the flow. The shape of mean velocity excess indicates momentum thickness of the flow and helps determine the spread angle of the jet. The normalized streamwise mean velocity excess at various downstream locations are presented in Fig. 2.11a. The term $U_e = \overline{u_1} - U_{co}$ denotes the mean streamwise velocity excess, $\overline{u_1(x_2)}$ the local mean velocity, $U_{co}$ the local mean co-flow velocity and $\Delta U_c$ the difference between local mean centerline velocity and local mean co-flow velocity. The mean streamwise velocity is observed to collapse to a self similar profile after a distance $x_1 > 7.5D_{jet}$, from the inlet. This shows good agreement with data from experiments on slot jets by Shestakov et al. [73] and plane jets by Gutmark and Wygnanski [74], and Ramaprian and Chandrasekhara [75]. Details of the setup and flow parameters of various experiments are presented in Table (2.3). Although the physical models used in this simulation differ from the experiment, the flow parameters and evolution can be compared as long as the Reynolds numbers are in similar range. In $x_2$ direction, the cross-steam velocity itself is used for mean velocity excess since $U_{co,x_2} = 0$. The cross-stream velocity profile also shows good agreement with experimental data.

The downstream growth of the decay of centerline velocity excess is presented in Fig. 2.12, where $\Delta U_0$ denotes the difference between mean centerline velocity and mean co-flow velocity at the inlet and $\Delta U_e$ denotes the difference between mean centerline velocity and mean co-flow velocity at downstream location. The centerline velocity decay is also observed to compare well with the experimental data of Shestakov et al. [73], Thomas and Prakash [76], and Hussain and Clark [77]. An inverse relationship between the downstream velocity decay and $x_1$ is obtained similar to the
DNS results from works of Stanley et al. [40].

\[
\left[ \frac{\Delta U_0}{\Delta U_c} \right]^2 = a_1 \left[ \frac{x_1}{D_{jet}} + a_2 \right],
\]

where \(a_1\) and \(a_2\) represent the slope and coefficient of curvefit, respectively. Table (2.2) presents comparison of these values with results from the aforementioned experiments.

### 2.9.3 Reynolds Stress on Jet Centerline

Downstream growth of the Reynolds stress on jet centerline is presented in Fig. 2.13. The Reynolds stress \((R_{ij} = \overline{u'_i u'_j} = \overline{\rho u'_i u'_j}/\overline{\rho})\) indicates the intensity of turbulence generated in the flow in the downstream direction. The normal Reynolds stresses \(R_{11}, R_{22}\) and \(R_{33}\) obtained from the DNS are compared against the experiments of Thomas and Prakash [76]. It is observed that the normal stress in \(x_1\) direction follows the experimental results closely. However, the trends in \(x_2\) and \(x_3\) directions are offset from the experimental results by \(x_1 \approx 5D_{jet}\). This is due to the fact that the transition of flow from laminar to turbulence in this DNS happens around \(x_1 \approx 10D_{jet}\) unlike the experiment where the natural transition to turbulence occurs around \(x_1 < 4D_{jet}\). However, in the fully turbulent region the trend of the normal Reynolds stress is observed to be in good agreement with the experiment.

### 2.10 Conclusions

First and second order statistics of the flow from DNS at atmospheric pressures show good agreement with results from the experimental studies. Structural evolution of the flow at larger pressures can be assumed to be qualitatively similar. This DNS can be used to extract the Filtered Mass Diffusion Function, Conditional Scalar Diffusion, the terms of the Reynolds stress budget and other statistics at various pressures.
Table 2.1: Summary of simulations and parameters from all cases considered.

<table>
<thead>
<tr>
<th>Run #</th>
<th>$P_0$ (atm)</th>
<th>Diffusion</th>
<th>Le</th>
<th>$Re_0$</th>
<th>EOS</th>
<th>$t^*$</th>
<th>$N_1 \times N_2 \times N_3$</th>
<th>CPU</th>
</tr>
</thead>
<tbody>
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<td>1</td>
<td>Generalized</td>
<td>$\neq 1$</td>
<td>850</td>
<td>Real</td>
<td>200</td>
<td>$240 \times 240 \times 60$</td>
<td>576</td>
</tr>
<tr>
<td>2</td>
<td>35</td>
<td>Generalized</td>
<td>$\neq 1$</td>
<td>850</td>
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<td>Real</td>
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<td>576</td>
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Table 2.2: Centerline mean velocity excess decay compared with several experiments and the physical parameters used in the experiments.

<table>
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<tr>
<th>Source</th>
<th>a1</th>
<th>a2</th>
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<th>$h/\theta$</th>
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<td>Thomas and Prakash</td>
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<td>8000</td>
<td>67</td>
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<td>30000</td>
<td>-</td>
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<td>Hussain and Clark</td>
<td>0.123</td>
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<td>32552</td>
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Table 2.2: Centerline mean velocity excess decay compared with several experiments and the physical parameters used in the experiments.
<table>
<thead>
<tr>
<th>Source</th>
<th>$Re_0$</th>
<th>$P_0(\text{atm})$</th>
<th>Species</th>
<th>Type</th>
<th>Flow profile</th>
<th>Velocity measurement</th>
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<td>Gutmark and Wygnanski</td>
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<td>Laser Doppler Anemometry (LDA)</td>
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<td>Particle Image Velocimetry, LDA</td>
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Table 2.3: Description of parameters used in experimental studies of planar and slot jets.
Figure 2.1: Computational Domain
Figure 2.2: Mean and Variance of velocity components $u_1$, $u_2$, and $u_3$ at $Re_0 = 850$ along the jet center-line at $x_1 = 20D_{jet}$.

Figure 2.3: Mean and Variance of velocity components $u_1$, $u_2$, and $u_3$ at $Re_0 = 1300$ along the jet center-line at $x_1 = 20D_{jet}$.
Figure 2.4: Flow evolution with various forcing frequencies at $Re = 850$ and $t^* = 50$. 

(a) $f = 0.2, \theta = \tan^{-1}\left(\frac{4\pi}{\nu}\right)$

(b) $f = 0.3, \theta = \tan^{-1}\left(\frac{4\pi}{\nu}\right)$

(c) $f = 0.4, \theta = \tan^{-1}\left(\frac{4\pi}{\nu}\right)$

(d) $f = 0.3, \theta = 1$
(a) Single side frequency spectrum of $R_{ij} = \langle u_i(x, t) u_j(x + r, t) \rangle$.

(b) Energy Spectral Density.

Figure 2.5: Turbulent velocity spectra obtained from the flow with sinusoidal forcing after application of high pass filter.
Figure 2.6: Density contours in minor and major jet planes at $P_0 = 1\ atm$, $Re_0 = 850$ and $t^* = 140$. 
Figure 2.7: Density contours in minor and major jet planes at $P_0 = 1 \text{atm}$, $Re_0 = 1300$ and $t^* = 140$. 

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Figure 2.8: Density contours in minor and major jet planes at $P_0 = 100\ atm$, $Re_0 = 850$ and $t^* = 140$. 
Figure 2.9: Density contours in minor and major jet planes at $P_0 = 100\, atm$, $Re_0 = 1300$ and $t^* = 140$. 
Figure 2.10: Instantaneous contour plot of mixture fraction at $P_0 = 100$ atm and $t^* = 180$. 

(a) $Re = 850$

(b) $Re = 1300$
Figure 2.11: Mean velocity profiles in slot jet.
Figure 2.12: Downstream growth of center-line mean velocity excess decay.
Figure 2.13: Downstream growth of the normal Reynolds stress.
Chapter 3

Subgrid Analysis

In LES, spatial filters with prescribed cutoff filter widths are applied to the governing equations in the physical space. As a result the flow characteristics at length scales larger than the filter widths are captured and those smaller than the filter widths are modeled. The governing equations and the modeling approaches used in LES are discussed in the following sections.

3.1 LES Governing Equations

A filtering operation of the form,
\[
\langle f(x,t) \rangle_l = \int_{-\infty}^{\infty} f(x',t)G(x',x)dx',
\]
(3.1)
is performed on the conservation (mass, momentum, energy, and scalar) equations. In the above equation \( G(x) \) denotes the filter function of width \( \Delta G \) and \( \langle f(x,t) \rangle_l \) represents the filtered value of variable \( f(x,t) \). The fluctuations of \( f(x,t) \) can then be obtained as \( f' = f - \langle f \rangle_l \). In variable density flows, a Favre filtering operation of form, \( \langle f(x,t) \rangle_L = \langle \rho f \rangle_l / \langle \rho \rangle_l \) is performed and the fluctuations are obtained as, \( f'' = f - \langle f \rangle_L \). A filter function that is spatially and temporally invariant \( (G(x',x) = G(x'-x)) \), with properties \( G(x) = G(-x) \), and \( \int_{-\infty}^{\infty} G(x)dx = 1 \), is chosen.

The resulting governing equations for LES can be written as,
\[
\frac{\partial \langle \rho \rangle_l}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial x_i} = 0,
\]
(3.2)
\[
\frac{\partial \langle \rho \rangle_l}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L}{\partial x_j} = - \frac{\partial \langle P \rangle_l}{\partial x_i} + \frac{\partial \langle \tau_{ij} \rangle_l}{\partial x_j} + \frac{\partial T_{ij}}{\partial x_j},
\]
(3.3)

\[
\frac{\partial \langle \rho \rangle_l \langle e \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle u_j \rangle_L}{\partial x_j} = - \frac{\partial \langle P \rangle_l \langle u_i \rangle_L}{\partial x_i} + \frac{\partial \langle \tau_{ij} \rangle_l \langle u_i \rangle_L}{\partial x_j} - \frac{\partial \langle Q_j \rangle_l}{\partial x_j} + \frac{\partial \langle \sum \alpha J_{i} \rangle_L}{\partial x_j} + \frac{\partial \langle S_{i} \rangle_l}{\partial x_j},
\]
(3.4)

\[
\frac{\partial \langle \rho \rangle_l \langle \phi_{\alpha} \rangle_L}{\partial t} + \frac{\partial \langle \rho \rangle_l \langle u_i \rangle_L \langle \phi_{\alpha} \rangle_L}{\partial x_j} = - \frac{\partial \langle J_{i}^{\alpha} \rangle_l}{\partial x_j} + \frac{\partial \langle M_{i}^{\alpha} \rangle_l}{\partial x_j} + \langle \rho S_{i} \rangle_l, \quad \alpha = Y_1...Y_N.
\]
(3.5)

\[
\langle P \rangle_l = \left\langle \frac{RT}{\bar{v}} - B_m \frac{A_m}{\bar{v}^2 + 2\tau B_m - B_m^2} \right\rangle_l
\]
(3.6)

In the above equations, \( \langle \rho \rangle_l \) represents the filtered density of fluid, \( \langle u_i \rangle_L \) the Favre filtered velocity in each coordinate direction, \( \langle P \rangle_l \) the filtered pressure, \( \langle \tau_{ij} \rangle_l \) the filtered viscous stress tensor, \( \langle \phi_{\alpha} \rangle_l \) the filtered scalar, \( \langle J_{i}^{\alpha} \rangle_l \) the filtered diffusion flux of species \( \alpha \), and \( \langle S_{i} \rangle_l \) the filtered chemical source term. The term \( T_{ij} = \langle \rho \rangle_l \langle (u_i u_j)_L - (u_i)_L (u_j)_L \rangle \), represents the unclosed sub-filter stress tensor, \( E_j = \langle \rho \rangle_l \langle (e_i u_j)_L - (e_i)_L (u_j)_L \rangle \) the unclosed sub-filter energy flux vector and \( M_{j}^{\alpha} = \langle \rho \rangle_l \langle (u_i \phi_{\alpha})_L - (u_i)_L \langle \phi_{\alpha} \rangle_L \rangle \), the unclosed sub-filter mass flux vector. In this work a grid based filtering is performed so the sub-filter terms henceforth will be referred to as subgrid terms. Modeling in LES of non-reacting flows is primarily associated with closure of the terms \( T_{ij}, E_j \) and \( M_{j}^{\alpha} \). Other subgrid terms such as those associated with the heat and mass flux vectors and the equation of state are typically neglected although can be significant [78, 79].

### 3.2 Functional Models

A functional model like the Smagorinsky model may be summarised as,

\[
T_{ij} - (\delta_{ij}/3)T_{kk} = -2(C_s \Delta_G)^2 \left| \bar{\tau} \right| s_{ij},
\]
(3.7)
where $\delta_{ij}$ represents the Kronecker delta function, $C_s$ the Smagorinsky constant and $s_{ij}$ the strain rate tensor. For variable density flows, a modified version of the model is proposed by Bardina et al. [80],

$$T_{ij} = -2C_R\langle \rho \rangle |\Delta G^1/2\langle (s_{ij})_L \rangle - \frac{1}{3}\langle s_{kk} \rangle_\ell \delta_{ij} \rangle + \frac{2}{3}C_l|\rho|\xi \delta_{ij},$$

$$\xi = |\langle u_{i}^* \rangle_L \langle u_{i}^* \rangle_L - \langle \langle u_{i}^* \rangle_L \rangle \langle \langle u_{i}^* \rangle_L \rangle |,$$

$$u_{i}^* = u_{i} - U_{ref,i},$$

where $\langle (s_{ij})_L \rangle$ represents the resolved strain rate tensor, $U_{ref,i}$ represents the reference velocity in each coordinate direction, the subscript $l'$ denotes a filter at secondary level such that $\Delta G' > \Delta G$, and $C_R, C_l$ represent the model constants. The subgrid energy and mass flux vectors in Eqs.(3.4,3.5) are closed using a diffusivity model.

$$E_i = -\gamma_t \frac{\partial \langle e_i \rangle_L}{\partial x_i},$$

$$M_{i}^{\alpha} = -\gamma_t \frac{\partial \langle \phi_{i} \rangle_L}{\partial x_i},$$

where $\gamma_t = \langle \rho \rangle \nu / S c_t$ represents the subgrid diffusivity with $\nu = C_R \Delta G^1/2$ and $S c_t$ represents the subgrid Schmidt number. Alternatively, the above terms may also be closed using a dynamic subgrid scale (SGS) model [81, 82, 83].

The modeling approach described here for the subgrid stress tensor, subgrid energy and mass flux vectors produce satisfactory results in LES of non-reacting flows. However, in reacting flows a functional model for the reaction source term ($S_{\alpha}$) can result in large errors. The reaction source term is highly non-linear and stochastic in nature. Thus, the model used to close this term must also have these properties. Deterministic models for reaction source terms may work for a small number of cases in very specific flows, but for highly compressible flows with large fluctuations in flow properties a different approach must be taken. A detailed survey of turbulent combustion models for LES of propulsive flow fields is presented in the works of Miller and Foster [84].

### 3.3 FMDF Based Modeling

The filtered mass density function (FMDF) method is a stochastic approach to modeling turbulent flows in LES. The FMDF method was proposed by Givi et al. [5, 6] and is based on the
PDF method for reactive flows proposed by Pope [4]. The idea of this method is to obtain a complete statistical description of the flow from a joint PDF defined for the velocity and scalars of the flow. A transport equation for this joint PDF is then derived, from which the statistical moments of the flow can be determined. The main advantage of this method is that the reaction source term in Eqs. (3.4, 3.5) is closed and requires no modeling. The FMDF method is similar to the PDF method except that the FMDF performs a Favre filtering operation on the PDF. For a scalar \( \phi(x, t) \), the FMDF \( (F_L) \) may be defined as,

\[
F_L(\psi; x, t) = \int_{-\infty}^{\infty} \rho(x', t) f[\psi, \phi(x', t)] G(x' - x) dx',
\]

where \( \delta \) represents a delta function and \( f[\psi, \phi(x, t)] \) represents the fine-grained density. The FMDF has property,

\[
\int_{-\infty}^{\infty} F_L(\psi; x, t) d\psi = \int_{-\infty}^{\infty} \rho(x', t) G(x' - x) dx' = \langle \rho(x, t) \rangle_L.
\]

The mass weighted conditional mean of a flow variable may then be obtained as,

\[
\langle Q(x, t) | \psi \rangle_L = \int_{-\infty}^{\infty} \rho(x', t) Q(x', t) f[\psi, \phi(x', t)] G(x' - x) dx' \over F_L(\psi; x, t).
\]

Some properties of this conditional mean are,

- for \( Q(x, t) = c \), \( \langle Q(x, t) | \psi \rangle_L = c \),
- for \( Q(x, t) = \tilde{Q}(\phi(x, t)) \), \( \langle Q(x, t) | \psi \rangle_L = \tilde{Q}(\psi) \),
- \( \int_{-\infty}^{\infty} \langle Q(x, t) | \psi \rangle_L F_L(\psi; x, t) d\psi = \langle \rho(x, t) \rangle_L \langle Q(x, t) \rangle_L \).

An exact transport equation for the scalar-FMDF can then derived following the procedure of Pope [4], Colucci et al. [5], Jaberi et al. [6]. The final form of FMDF transport equation may be expressed as,

\[
\frac{\partial F_L}{\partial t} + \frac{\partial}{\partial x_i} \left[ \langle u_i \psi \rangle L \right] F_L = \frac{\partial}{\partial \psi_\alpha} \left[ \left( \frac{1}{\rho} \frac{\partial J_\alpha}{\partial x_i} \right) \langle \psi \rangle L \right] F_L - \frac{\partial [S_\alpha F_L]}{\partial \psi_\alpha},
\]

The chemical reaction source term in the above equation is closed. However, two new terms appear that remain unclosed: \( \langle u_i | \psi \rangle_L \), in the second term on the left hand side of the equation is called subgrid scalar convection and represents the motion of scalars at the subgrid scales due to the flow...
velocity. This term is typically modeled using a functional model. It may be decomposed as,

\[
\langle u_i | \psi \rangle_L F_L = \langle u_i \rangle_L F_L + [\langle u_i | \psi \rangle_L - \langle u_i \rangle_L] F_L,
\]

(3.14)

where the term \([\langle u_i | \psi \rangle_L - \langle u_i \rangle_L] F_L\) represents the SGS convective flux and may be modeled in a manner similar to the SGS mass flux term in Eq.(3.9):

\[
[\langle u_i | \psi \rangle_L - \langle u_i \rangle_L] F_L = -\gamma_t \frac{\partial (F_L/\langle \rho \rangle_i)}{\partial x_i}.
\]

(3.15)

Equation (3.13) can then be rewritten as,

\[
\frac{\partial F_L}{\partial t} + \frac{\partial[(u_i) L F_L]}{\partial x_i} = \frac{\partial}{\partial x_i} \left[ (\gamma + \gamma_t) \frac{\partial (F_L/\langle \rho \rangle_i)}{\partial x_i} \right] + \frac{\partial}{\partial \psi} \left[ \left\langle \left. \frac{1}{\rho} \frac{\partial J_\alpha}{\partial x_i} \right| \psi \right\rangle_L - S_\alpha \right] F_L.
\]

(3.16)

This transport equation is solved using a Lagrangian Monte Carlo method where the spatial transport is governed by a stochastic differential equation and the composition transport is solved in a mesh free Lagrangian setup simultaneously. \(\left\langle \left. \frac{1}{\rho} \frac{\partial J_\alpha}{\partial x_i} \right| \psi \right\rangle_L\) in the second term on the right hand side of the equation is the conditional scalar diffusion (CSD). This remains as the last unknown term in this transport equation but treatment of this term using a functional approach is not straightforward. It represents the effects of molecular transport (diffusion) in physical space and molecular mixing in composition space. The spatial transport of a Lagrangian particle in subgrid space is governed by a Wiener process (random walk) that uses a single diffusion coefficient while the composition change within subgrid space is modeled by a molecular mixing model. The spatial transport of FMDF can be expressed as,

\[
\frac{dX_i}{dt} = D_i + E_i \frac{dW}{dt},
\]

(3.17)

where \(X_i\) represents the position of a stochastic particle in the Lagrangian space, and \(D_i, E_i\) represent the drift and diffusion coefficients of Wiener process \(W_i\). The composition evolution of a Lagrangian fluid element \((\phi_\alpha)\) can be written as,

\[
\frac{d\phi_\alpha}{dt} = \Theta_\alpha - S_\alpha,
\]

(3.18)

with \(\Theta_\alpha = \left\langle \left. \frac{1}{\rho} \frac{\partial J_\alpha}{\partial x_i} \right| \psi \right\rangle_L\). A few mixing models that stem from different physical concepts have been proposed for treatment of this term. The following section briefly discusses the Interaction by
3.3.1 Interaction by Exchange of Mean

The Interaction by Exchange of Mean (IEM) [85] otherwise known as the Linear Mean Square Estimation (LMSE) [86] is one of the simplest deterministic models that describes the phenomena of mixing at the subgrid scale. The composition evolution using this model is given by,

$$\frac{d\phi_\alpha}{dt} = \Theta_\alpha = \Omega_m (\psi_i - \langle \psi \rangle_l), \quad (3.19)$$

where $\langle \psi \rangle_l$ represents the volume average of a scalar $\psi$ and $\psi_i$ represents the instantaneous value of the scalar within the filter confines. In essence, the model causes the composition of a Lagrangian particle within a given filter volume to relax towards the mean value at a rate $\Omega_m \sim \varepsilon/K$. The term $\Omega_m$ represents the mixing frequency, $k$ the turbulent kinetic energy and $\varepsilon$ its dissipation rate. The main advantage of this model is its simplicity and ease of implementation. The mixing frequency can be determined from the parameters measured in the simulation using a dimensional analysis.

Jaberi et al. [6] proposed an expression for $\Omega_m(x,t)$ as,

$$\Omega_m = C_\Omega \frac{(\gamma + \gamma_t)}{\left(\langle \rho \rangle_l \Delta G^2 \right)}, \quad (3.20)$$

In this equation, $\gamma$ represents the molecular diffusivity, $\gamma_t = \langle \rho \rangle_l \frac{C_R \rho \Delta G^2}{Sc_t}$ the subgrid scalar diffusivity, $\langle \rho \rangle_l$ the filtered density, $\Delta G$ the filter width, $Sc_t$ the subgrid Schmidt number, $C_R, C_\Omega$ the model constants and $\xi$ is obtained by method similar to that in Eq.(3.8). The dimensions of mixing frequency is $[1/s]$. A preliminary test on applicability of the IEM model for a general mixing case was performed as a part of this study. The average of the Laplacian of an arbitrary function ($f(x)$) conditioned with the spatial variable ($\langle \nabla^2 f|x \rangle$) is obtained and compared against the fluctuation of the function itself ($f' = f - \langle f \rangle$). The results in Fig. 3.17 indicate a good closure of conditional averages using the IEM model. The conditional scalar diffusion is local in composition space but the IEM model is local only in physical space. Thus, for dispersed flows that have large spatial variation of concentration, the IEM model may not be well suited.
3.3.1.1 IECM

An improvement to the IEM model called Interaction by Exchange of Conditional Mean (IECM) was proposed by Pope [87] and Fox [88] to overcome the dispersion inconsistency [89]. In this model, instead of standard averaging of the scalar (volume average within filter), a velocity conditioned average of the scalar is used. In the IEM model, the particles that have similar spatial positions interact with each other but in the IECM model the particles that have similar velocities interact with each other. Physically it represents interaction of particles that belong to the same eddy. Thus in dispersed turbulent flows, the IECM model is expected to be more accurate than IEM in predicting the SGS mixing phenomena. The IECM model can be expressed as,

\[ \Theta_\alpha = \Omega_m (\phi_i - \langle \phi | U \rangle_l). \] (3.21)

However, this model is also non-local in composition space.

3.3.1.2 IEM + Mean Drift

Another modification to the IEM model called the IEM plus mean drift was proposed by McDermott and Pope [90]. In this model, the composition transport is governed by the IEM model but the transport in physical space is modeled using a mean drift term instead of a random walk. Since the random walk method uses a single diffusion coefficient, it does not take into account the effects of differential diffusion in the flow. The model may be expressed as,

\[ \frac{d\phi_\alpha}{dt} = \Omega_m (\psi_i - \langle \psi \rangle_l) + \left[ \frac{1}{\langle \rho \rangle_i} \frac{\partial}{\partial x_j} \left( \langle \rho \rangle_i \langle \gamma \rangle_l \frac{\partial \langle \phi_\alpha \rangle_l}{\partial x_j} \right) \right]. \] (3.22)

The mean drift term in the above equation is based on the standard Fickian diffusion.

3.3.2 Modified Curl

The modified curl (MC) model proposed by Janicka et al. [91] is a particle interaction model based on Curl’s [92] model. For equally weighted particles, pairs of particles are randomly selected
from an ensemble and their compositions are changed as,

\[
\phi_{i,\text{new}} = \phi_i + 0.5R_{ij}(\phi_j - \phi_i),
\]

\[
\phi_{j,\text{new}} = \phi_j + 0.5R_{ij}(\phi_i - \phi_j).
\]

The model for conditional diffusion can be re-written as,

\[
\Theta_\alpha = \Omega_m R_{ij} C_{MC}(\phi_c - \phi_j),
\]

\[
\phi_c = \frac{w_i \phi_i + w_j \phi_j}{w_i + w_j}
\]

where \(\phi_i, \phi_j\) represent particles from the ensemble, \(w_i, w_j\) represents the weights of the particles, \(R_{ij}\) represents a uniformly distributed random number, \(C_{MC}\) represents the model constant and \(\Omega_m\) is mixing frequency similar to one used in the IEM model. A model for unequal weights was developed by Nooren et al. [93] but effective working of model depends on distribution of particle weights. Unlike the IEM, the MC model is stochastic in nature but is still local in physical space and not in composition space.

### 3.3.3 Mapping Closure

The Mapping Closure (MAPPING) model for CSD was formulated by Kraichnan [94] and Chen et al. [95]. The model suggests that the scalars in turbulent flows follow an assumed distribution. A model for mixing of particles that follow this distribution is then derived. For unequally weighted particles, the model proposed by Pope [96] maps the composition space of a single scalar with a Gaussian reference field. The scalar evolution of particles can be written as,

\[
\frac{d\phi_1}{dt} = -C_{map} \Omega_m [B_{1+\frac{1}{2}} (\phi_2 - \phi_1)],
\]

\[
\frac{d\phi_i}{dt} = C_{map} \Omega_m [B_{i+\frac{1}{2}} (\phi_{i+1} - \phi_i) - B_{i-\frac{1}{2}} (\phi_i - \phi_{i-1})]; i = 2, \ldots, N_p - 1,
\]

\[
\frac{d\phi_{N_p}}{dt} = -C_{map} \Omega_m [B_{N_p-\frac{1}{2}} (\phi_{N_p} - \phi_{N_p-1})],
\]

where \(C_{map}\) represents the model constant and \(\Omega_m\) the mixing frequency. The scalars \(\phi_i\) in the equations are sorted from the smallest to largest values (\(\phi_i < \phi_{i+1}\)). The coefficients \(B\)'s are defined
as,

\[
B_{i+\frac{1}{2}} = \frac{N_p g(\eta_{i+\frac{1}{2}})}{\eta_{i+1} - \eta_i},
\]

\[
B_{i-\frac{1}{2}} = \frac{N_p g(\eta_{i-\frac{1}{2}})}{\eta_i - \eta_{i-1}}.
\]

(3.26)

\[N_p\] in this equation represents the total number of particles and \(g(\eta)\) represents a standard Gaussian PDF with sample space coordinate \(\eta\). \(\eta\) is defined as,

\[
\eta_{i+\frac{1}{2}} = G^{-1}(p_i),
\]

\[
\eta_i = G^{-1}(p_{i-\frac{1}{2}}),
\]

\[
\delta \eta_i = \eta_{i+\frac{1}{2}} - \eta_i,
\]

(3.27)

where \(\delta \eta_i\) is the half step difference such that \(\eta_{i+1} = \eta_{i+\frac{1}{2}} + \delta \eta_i\) and \(G^{-1}\) represents the inverse cumulative density function corresponding to the PDF \(g\). The arguments \(p\)'s are defined as,

\[
p_{i+\frac{1}{2}} = \frac{\sum_{j=1}^{i} w_j - 0.5w_i}{W},
\]

\[p_i = \sum_{j=1}^{i} w_j/W.\]

(3.28)

\(W\) in the equation above represents the sum of weights of all particles in the ensemble. The boundary values of coefficients are given as,

\[
B_{1+\frac{1}{2}} = \frac{N_p g(\eta_{1+\frac{1}{2}})}{\eta_2 - \eta_1},
\]

\[
B_{N_p-\frac{1}{2}} = \frac{N_p g(\eta_{N_p-\frac{1}{2}})}{\eta_{N_p} - \eta_{N_p-1}},
\]

(3.29)

\[\eta_{1+\frac{1}{2}} = \eta_1 + \delta \eta_1,
\]

\[\eta_{N-\frac{1}{2}} = \eta_{i+\frac{1}{2}} \mid i = N_p - 1.\]

The mapping closure model preserves the mean and variance decay. Since the scalars are sorted, the resulting model is local in composition space. However, the model is applicable only to a single scalar. An extension of this model to multiple scalars called Euclidean Minimum Spanning Tree (EMST) was proposed by Pope [97]. The EMST model forms a minimum spanning tree based on composition of particles in an ensemble. The lengths of the vertices of the spanning tree are dependent on the
weights, and age properties of particles which enables treatment of multiple scalars. The mixing is then performed for particles that lie in the minimum spanning tree. This algorithm is more complex and requires more computational time compared to a mapping closure model, but preserves the localness property for mixing. This model however, does not satisfy the independence and linearity properties [98]. Another model called Shadow-Position Mixing (SPM) proposed by Pope [89], relaxes the instantaneous scalar composition within a filter to a shadow position rather than the cell average as in the IEM model. This model is relatively new and only limited testing has been performed on this.

3.4 Measurement of Subgrid Terms

The subgrid flow phenomena that is modeled in LES can be calculated from DNS by breaking down the DNS domain and performing volume averages of flow properties within each of the smaller domains.

\[ L_i = N_i \Delta x_i = N_i' \Delta x_i', \]
\[ \Delta x_i' \gg \Delta x_i, \]
\[ N_i >> N_i', \]  \hspace{1cm} (3.30)

where \( N_i, N_i' \) represent the number of grid points, and \( \Delta x_i, \Delta x_i' \) represent the grid size in a coordinate direction used in DNS and LES, respectively. The subgrid flow characteristics (filtered mass density function, conditional scalar diffusion) are directly computed from DNS and compared against the SGS models to evaluate the effectiveness of closure at large pressures with a generalized diffusion model. In molecular mixing models, the effects of chemical source term on CSD and vice-versa is neglected. Studies performed by Liu and Tong [99, 100] on sensitivity of reaction source term on mixing suggest that mixing models based on non-reactive scalar can be used to model mixing of reactive scalars as well. The mixing models presented in this section are validated using DNS of mixing jets of heptane-air and heptane-oxygen. Simulation of mixing of heptane-oxygen is performed to evaluate the performance of mixing models for binary mixing cases.
3.4.1 Filtered Mass Density Function

The FMDF represents the distribution of fluctuations of subgrid scalars. Unlike a PDF in RANS, the FMDF is stochastic in nature. The PDF in RANS characterizes fluctuations over various flow realizations, but the FMDF characterizes the instantaneous subgrid fluctuations. The mean of LES-FMDF is equal to the RANS-PDF when the filter width tends to zero [101]. Inspite of the differences between the two, the FMDF has all the mathematical properties of a PDF. Thus in LES, the FMDF may be used to obtain all the statistics of the flow. In FMDF transport equation the effect of CSD is to change the shape of the FMDF. Without this term, the FMDF would remain unchanged. The model for CSD is determined to be the largest source of uncertainty in FMDF calculation. The FMDF for a scalar can be obtained from the DNS data by applying a spatial filter of appropriate width to the scalar variable in the DNS code, extracting the filtered scalar at various points in the flow and obtaining the PDF of the filtered scalar. The FMDF of mixture fraction obtained from the DNS near the jet centerline is presented Figs. 3.1-3.8. The FMDF is extracted from the DNS after the flow has reached a statistically stationary state.

The mixture fraction definition used in this work may be expressed as,

\[ \phi = \frac{sY_f - Y_o + Y_o^0}{Y_f^0 + Y_o^0}, \]  

(3.31)

where \( s \) represents the stoichiometric coefficient, \( Y_f, Y_o \) represent the instantaneous mass fractions and \( Y_f^0, Y_o^0 \) represent the initial free stream mass fractions of fuel and oxidizer, respectively. For heptane-air mixture, the mass fraction of oxidizer indicates sum of mass fractions of oxygen and nitrogen. The mixture fraction may take a value between 0 (pure oxidizer) and 1 (pure fuel) indicating the proportion of fuel within the mixture. For multi-species mixture, the mixture fraction should ideally be defined in terms of elemental mass fraction [62]. However, for pure mixing cases, the definition in Eq.(3.31) is sufficient.

The shapes of the FMDF describe the distribution of the SGS fluctuations. When the mixture fraction is highly segregated, the shape of FMDF is bimodal, else it is unimodal indicating high concentrations of either fuel or oxidizer [102, 103]. In highly dispersed flows, multimodal shapes may also be observed. In non-premixed flows, the regions close to the nozzle along the jet centerline and freestream typically have high concentrations of fuel and oxidizer, respectively. In simulations at atmospheric pressures with the standard Fickian diffusion model, the FMDF is observed to be
predominantly unimodal at the jet centerline. At the shear region, a bimodal shape is observed. The FMDF in Figs. 3.7-3.8 indicate a fuel rich zone along the jet centerline even at long simulation run times. The FMDF at $P_0 = 100\text{atm}$ with the Fickian diffusion model, is observed to be similar to that at $P_0 = 1\text{atm}$ indicating no significant change with pressure. From Fig. 3.1 it is observed that at atmospheric pressures with the generalized diffusion model, the FMDF is bimodal. The bimodal shape of FMDF at $P_0 = 1\text{atm}$ with the generalized diffusion model is seen to become more segregated with increase in Reynolds number ($Re_0 = 1300$) as seen in Fig. 3.4. With increase in pressure, the FMDF in Figs. 3.2 and 3.3 are observed to become multimodal and $\phi$ is observed to shift towards the oxidizer rich regime. This indicates intensification of mixing and increase in rate of diffusion of fuel with increase in pressure. The change of rate of diffusion with pressure will be discussed in detail in the Section (3.4.2). The FMDF at high pressures at $Re_0 = 1300$ exhibit similar patterns of highly segregated multimodal shapes as indicated in Figs. 3.5-3.6. With the generalized diffusion model [Eq. 2.8], a significant change in FMDF is observed especially at $P_0 > 1\text{atm}$. The generalized diffusion model takes into account the diffusion due to concentration and pressure gradients which become very significant at large pressures.

3.4.2 Conditional Scalar Diffusion

CSD in Eq.(3.16) indicates the expected value of diffusion rate of a scalar at a particular value of mixture fraction. Physically it represents the change of composition of particles within a subgrid volume. The rate of diffusion of particles with varying compositions is different, to bring down the gradients in said composition. In turbulent flows, this term is time dependent since the composition within subgrid volume changes with flow instantaneously. CSD therefore has a significant effect on the FMDF and needs to be modeled accurately. A major advantage of DNS is that it allows calculation of CSD directly from the code.

3.4.2.1 Transport Equation for Mixture Fraction

For numerical simulations with standard the Fickian diffusion model, the scalar diffusion rate is given by,

$$\left( \frac{\partial J_j^\phi}{\partial x_j} \right)_F = \frac{\partial}{\partial x_j} \left[ \rho \gamma \frac{\partial \phi}{\partial x_j} \right],$$

(3.32)
where \( \gamma \) represents the Fickian diffusion coefficient. However, for DNS with generalized diffusion models (without an effective diffusion coefficient) a transport equation for mixture fraction is required to obtain the scalar diffusion rate. In Eq. (3.31) the stoichiometric coefficient \( s = 1 \), for pure mixing (non-reacting) flows. Thus it may be rewritten as,

\[
Y_f - Y_o = \phi (Y_f^0 + Y_o^0) - Y_o^0. \tag{3.33}
\]

The transport equations for fuel and oxidizer [Eq. (2.4)] are expressed as,

\[
\frac{\partial}{\partial t} (\rho Y_f) + \frac{\partial}{\partial x_j} (\rho u_j Y_f + J_{j,f}) = S_Y, \tag{3.34}
\]

\[
\frac{\partial}{\partial t} (\rho Y_o) + \frac{\partial}{\partial x_j} (\rho u_j Y_o + J_{j,o}) = S_Y. \tag{3.35}
\]

For pure mixing flows, the source terms \( S_Y = S_Y = 0 \). Subtracting Eqs. (3.35) from (3.34) gives,

\[
\frac{\partial \rho}{\partial t} (Y_f - Y_o) + \frac{\partial}{\partial x_j} (\rho u_j (Y_f - Y_o) + J_{j,f} - J_{j,o}) = 0. \tag{3.36}
\]

Substituting the mixture fraction definition from Eq. (3.33) into Eq. (3.36) gives,

\[
\frac{\partial \rho}{\partial t} (\phi (Y_f^0 + Y_o^0) - Y_o^0) + \frac{\partial}{\partial x_j} \left[ \rho u_j [\phi (Y_f^0 + Y_o^0) - Y_o^0] + J_{j,f} - J_{j,o} \right] = 0,
\]

\[
(Y_f^0 + Y_o^0) \frac{\partial \rho \phi}{\partial t} - Y_o^0 \left( \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j \phi) \right) + (Y_f^0 + Y_o^0) \frac{\partial}{\partial x_j} (\rho u_j \phi) + \frac{\partial}{\partial x_j} (J_{j,f} - J_{j,o}) = 0. \tag{3.37}
\]

The second term in the above equation results in the continuity equation. The final transport equation for mixture fraction can then be written as,

\[
\frac{\partial \rho \phi}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j \phi) + \frac{1}{(Y_f^0 + Y_o^0)} \frac{\partial}{\partial x_j} (J_{j,f} - J_{j,o}) = 0, \tag{3.38}
\]

where the scalar diffusion rate for mixture fraction is expressed as,

\[
\left( \frac{\partial J_{j}^0}{\partial x_j} \right)_G = \left[ \frac{1}{(Y_f^0 + Y_o^0)} \frac{\partial}{\partial x_j} (J_{j,f} - J_{j,o}) \right]. \tag{3.39}
\]
3.4.2.2 CSD Measurement from DNS

To measure the CSD, the scalar diffusion rate of mixture fraction is calculated throughout the domain in the DNS code. At a spatial location within the flow, an appropriate filter size is chosen ($\Delta_f = r\Delta x_i$, where $r$ is the radius of sphere for a spherical filter or half the length of a side for a cubic filter) for measurement of subgrid terms. A filter of volume defined by the filter size is then constructed ($V_f = \frac{4}{3}\pi\Delta_f^3$, for spherical filter and $V_f = \Delta^3_f$ for cubic filter). The terms (scalar diffusion and mixture fraction) at grid nodes within the filter confines are then extracted. These terms will be referred to, as subgrid (sub-filter) particles in rest of the work. The averages of scalar diffusion rate of the subgrid particles conditioned at various mixture fractions are then obtained. In this work a cubic filter is used. A similar procedure may be applied to obtain conditional averages of other scalars or scalar diffusion conditioned at different values of other variables (velocity conditioned diffusion, velocity-scalar conditioned diffusion). CSD at various instants of time measured from DNS at pressures of 1 atm, 35 atm and 100 atm with the generalized and the simplified Fickian diffusion model [Eq. 3.32] are presented in Figs. 3.9-3.16. For analysis and validation of models, statistically stationary DNS data is used.

A generally observed trend is, high rates of diffusion in the fuel and oxidizer rich zones and low rates of diffusion around $\phi = 0.5$. CSD is stochastic in nature but the variation in shape and magnitude of the term with respect to time is observed to be small. The absolute magnitude of CSD is observed to increase non-linearly with increase in ambient pressure.

3.5 Conditional Scalar Diffusion Modeling

The models for CSD discussed in Section (3.3.1) have been evaluated against DNS at various pressures with the generalized and Fickian diffusion models. Least-squares curve fitting method has been applied and the modeling constants have been calibrated to best fit the data obtained from DNS. The curve fits of the IEM, MC and MAPPING models for CSD are presented in Figs. 3.18-3.27.

3.5.1 Interaction by Exchange of Mean

The IEM model for mixture fraction ($\phi$) is expressed as,

$$\left\langle \frac{1}{\rho} \frac{\partial f_\alpha}{\partial x_i} \right\rangle_t = \Theta_\alpha = C_{IEM} \Omega_m(\phi_i - \langle \phi \rangle_i). \quad (3.40)$$
The parameters for mixing frequency \( (\Omega_m) \) defined in Eq.(3.20) are chosen as \( C_\Omega = 4 \), \( C_R = 0.013 \), \( \Delta_G = 12 \) and \( Sc_l = 0.7 \). The parameters are obtained from the works of Jaberi et al. [6]. The IEM model fits CSD linearly. The trends predicted by the model is observed to be exact for flows at atmospheric pressures with both ideal and real gas equations of state, and the standard Fickian and generalized diffusion models. However, at \( P_0 = 100 \text{atm} \) with the Fickian diffusion model, the IEM model over-predicts the CSD by a factor of 10. Similar trends are observed in flows at \( P_0 > 1 \text{atm} \) with the generalized diffusion model. The reason for the difference between the DNS data and model is determined to be the mixing frequency \( (\Omega_m) \). The mixing frequency is observed to be over-predicted by a factor of 10 or larger in flows at high pressures with the generalized diffusion model and under-predicted by a factor of 10 in flows at high pressure with the Fickian diffusion model. The mixing frequencies for various test cases are presented in Table (3.1). Variation of mixing frequency with pressure will be discussed in Section (3.5.4).

The curve fits of IECM model for CSD is presented in Figs. 3.28-3.33. With the corrected mixing frequencies (from the IEM model), the trends predicted by IECM model are qualitatively similar to that of the CSD. Although the curve fit is not exact, the norms of residuals of the model and DNS data presented in Table (3.2) are comparable.

### 3.5.2 Modified Curl

The modified curl model presented in Section (3.3.2) is a stochastic particle interaction model. The model constant in Eq.(3.24) is determined to be \( C_{MC} = 1 \) for flows at high pressures but for flow at atmospheric pressure with the generalized diffusion the model constant is determined to be \( C_{MC} = 2 \). Without the uniformly distributed random number \( R_{ij} \), the MC model fits the CSD curve linearly. The term \( R_{ij} \) causes interaction of random particles within an ensemble thereby producing a good curve fit for CSD. However, random selection of particles from an ensemble for mixing is not physical as interaction is dependent on closeness of particles in physical and composition space. Thus in turbulent flows with large fluctuations in density, temperature and scalars the MC model may not accurately predict the CSD. The randomness factor added to the model introduces an artificial fluctuation in the trend of the model that may not be representative of the physical phenomenon. From Figs. 3.18-3.27 it is observed that the model follows the general trend of CSD but tends to over-predict the DNS data. At atmospheric pressures the model predicts a trend similar to the DNS data but higher pressures the slope of model data is observed to be smaller than that.
of the CSD.

### 3.5.3 Mapping Closure

The mapping closure model presented in Section (3.3.3) is conceptually an improvement over the IEM and MC models. In this model the scalars within an ensemble are initially sorted and then mixed. This preserves the localness property of the model in composition space. In turbulent flows, particles with similar compositions tend to be local in physical space as well. The modeling constants ($C_{map}$) for various cases are presented in Table (3.3). The curve fits of model in Figs. 3.18-3.27 suggest that the MAPPING model does not strictly follow the trend of CSD. The slope of linear curve fit of model data is much smaller than that of CSD. This suggests that the model under-predicts the average conditional diffusion. However, at specific mixture fractions, the curve fit is representative of the actual phenomena. The small magnitude of slope of model data is a result of mixing of particles that are local within a composition space (due to sorted values of the scalar). However, if the scalars are unsorted, the trends predicted by the model are very similar to that of CSD as observed in Figs. 3.34-3.37. The curve fits of MAPPING model with unsorted scalar is similar to that of Modified Curl model. Although the curve fit in this case is accurate, it is not physical. The idea of MAPPING model for single scalar is extended to include multiple scalars in the EMST model. Evaluation of EMST model is not included in this work. The reader is referred to the work of Ma [98] for detailed evaluation of EMST model at high pressures with a generalized diffusion model for temporally evolving turbulent reacting flows.

### 3.5.4 Mixing Frequency

The mixing frequency is a common factor in all molecular mixing models. It represents the rate of change of composition of particles within a subgrid volume. Although different models stem from different concepts of particle interaction, the rate of mixing in each model remains the same. Additional modeling constants may be used in different models to fit the data to experimental results. In each of the aforementioned models, the largest source of uncertainty (in curve fitting DNS data) is determined to be the mixing frequency. The form of mixing frequency used in this work
may be expressed as,

\[
\Omega_m = C_\Omega \left[ \gamma + \left( \frac{\langle \rho \rangle_{i} \Delta G_S \sqrt{\xi} }{ \langle \rho \rangle_{i} \Delta^2_G } \right) \right],
\]

\[
\xi = |\langle u^i_l \rangle_L \langle u^i_l \rangle_L - \langle \langle u^i_l \rangle_L \rangle_{L'} \langle \langle u^i_l \rangle_L \rangle_{L'}|,
\]

\[
u^i = u^i - U_{ref,i}.
\]

This form is directly applicable only to flows at atmospheric pressures with the standard Fickian diffusion model. Even in the case of flow with the Fickian diffusion model at \( P_0 = 100 \text{atm} \), the \( \Omega_m \) calculated is off from the calibrated value by a factor of 10. This difference is more pronounced in flows that use a generalized diffusion model especially at large pressures. The source of the difference is determined to be the diffusivity \( \gamma \) (constant for Fickian diffusion). At atmospheric pressures, the rates of diffusion in flows with the generalized and Fickian diffusion models are observed to be similar. This rate is observed to deviate at larger pressures. Thus, a deviation factor for a generalized diffusion model may be obtained from the two rates. This may be expressed as,

\[
\gamma_{dev} = \left( \frac{\partial J^\phi}{\partial x^j} \right)_{G G}.
\]

At atmospheric pressures, the deviation term is almost constant (\( \gamma_{dev} \approx \gamma \)). However, at large pressures when cross-diffusion effects become more significant, the standard Fickian diffusion model with constant diffusivity tends to over-predict the rate of diffusion by a large factor. Thus \( \gamma_{dev} \) becomes crucial in case of flows at \( P_0 > 1 \text{atm} \). In this work, \( \gamma_{dev} \) is used instead of \( \gamma \) in Eq (3.41) to calculate \( \Omega_m \). Variation of parameters of mixing frequency (\( \Omega_m = f(\gamma, \langle \rho \rangle_{i}, 1/\Delta^2_G, \sqrt{\xi}) \)) with ambient pressure is presented in Figs. 3.38-3.43. At both Reynolds numbers the filtered density is observed to vary linearly with pressure irrespective of the diffusion model. The magnitude of variation of factor \( \xi \) over the large range of pressures is observed to be insignificant (\( \Delta \xi / \Delta P_0 < 0.1 \)). Although the magnitude of \( 1/\Delta^2_G \) is significantly high, it is independent of the physics of the flow and is the same for all the cases. Thus the factor that most significantly affects the mixing frequency is determined to be \( \gamma_{dev} \). Thus for accurate modeling, an effective diffusion coefficient for the generalized diffusion model is required. A species-specific effective diffusion coefficient for a generalized diffusion model was derived by Ma [98]. In his work, the generalized diffusion model for
a species \( \alpha \), \((\gamma^\alpha_{j,G})\) is approximated to a model diffusion term of form \( \gamma^\alpha_{eff} \partial Y^\alpha \partial x_j \). A least square error method is then applied to the data to obtain an effective diffusion coefficient of form, 

\[
\gamma^\alpha_{eff} = \frac{J^\alpha_{j,G} \partial Y^\alpha}{\rho \partial Y^\alpha \partial x_j}. \tag{3.43}
\]

An effective Schmidt number for generalized diffusion models was also proposed,

\[
Sc^\alpha_{eff} = \frac{\mu}{\rho \gamma^\alpha_{eff}}. \tag{3.44}
\]

The readers are referred to the work of Ma [98] for a detailed analysis of molecular mixing models with the effective diffusion coefficient for generalized diffusion models at high pressures. The new model constants \((C_{\Omega,new})\) for mixing frequency for various cases considered are presented in Table (3.1). These modeling constants are applicable when the deviation factor \((\gamma_{dev})\) is used instead of an effective diffusion coefficient \((\gamma_{eff})\) to calculate \(\Omega_m\) in flows with a generalized diffusion model.

The mixing frequency for turbulent flows can also be approximated by,

\[
\Omega_m = C_{k-\epsilon} \frac{\tau}{k}. \tag{3.45}
\]

In this equation, \(\tau\) and \(k\) represent the mean rate of dissipation and mean turbulent kinetic energy, respectively. The mixing frequency is approximated from the mean rate at which the turbulent kinetic energy of the flow is dissipated. Assuming a particle interaction mechanism similar to the IEM model (composition relaxation towards the mean) takes place within a subgrid volume, a conditionally averaged mixing frequency is determined.

\[
\langle \Omega_m | \phi \rangle_l = \frac{\langle \frac{1}{\rho} \frac{\partial j^\alpha}{\partial x_j} | \phi \rangle_l}{\phi_l - \langle \phi \rangle_l}. \tag{3.46}
\]

In this equation, \(\langle \Omega_m | \phi \rangle_l\) indicates the rates of mixing of particles and their corresponding compositions. This is compared against a conditional average of second invariant of strain tensor \(\langle Q_S | \phi \rangle_l\) obtained from the DNS. This term \(Q_S = II(s_{ij}) = -\frac{1}{2} s_{ij}s_{ij}\) is proportional to the local rate of viscous dissipation of kinetic energy [104]. From Figs. 3.44-3.46, it is observed that the general trend of \(\langle \Omega_m | \phi \rangle_l\) is similar to that of \(\langle Q_S | \phi \rangle_l\) (regions of high / low rates of viscous dissipation correspond to high / low rates of mixing frequency). This indicates a direct proportionality of the
mixing frequency with the rate of viscous dissipation. In many physical flows, the mechanism of the IEM may not be directly applicable but a similar trend may be observed.

In this work, the mean turbulent kinetic energy and dissipation rates are measured directly from the DNS at various pressures. This is discussed in detail in Section (4.3.2.2). The model constants $C_{k-\epsilon}$ for the corrected mixing frequencies are presented in Table (3.4). $C_{k-\epsilon}$ in most cases determined to be approximately 1. This suggests that, in LES with a generalized diffusion model, this form may be used as an alternate method to determine the mixing frequency.

$$\Omega_m \approx \frac{\epsilon_{SGS}}{k_{SGS}},$$
$$k_{SGS} = \frac{1}{2} u'' u'',$$
$$\epsilon_{SGS} = \nu \left( \frac{\partial u_i \partial u_i}{\partial x_j \partial x_j} - \frac{\partial \bar{u} \partial \bar{u}}{\partial x_j \partial x_j} \right).$$

(3.47)

However, evaluation of mixing frequency with the subgrid scale dissipation rate and kinetic energy obtained from LES has not been performed in this work. This can be evaluated as part of future work.

### 3.6 Conclusions

For LES of reacting flows, the FMDF method is one of the best choices since it avoids modeling of the reacting source term. However, in the LES-FMDF method, the accuracy of the simulation is highly dependent on the molecular mixing model used for the conditional scalar diffusion. Each of the models discussed in this work have some advantages and drawbacks but are directly applicable to a large range of flows at atmospheric pressures. However, at larger pressures, a significant deviation from the DNS results is observed. The cause for this deviation is determined to be the diffusivity term in the mixing frequency used by the models. At large pressures, the mixing frequency is under-predicted when a constant diffusivity is used and over-predicted when a deviation factor is used. The ideal solution is an effective diffusivity term for generalized diffusion models or determination of ratio of mean dissipation rate and mean turbulent kinetic energy from the flow. Although evaluation of mixing models is performed with DNS of non-reacting flows, the results are still applicable to LES of reacting flows (that use the IEM, MC, MAPPING models for FMDF).
<table>
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<th>$Re_0$</th>
<th>EOS</th>
<th>Diffusion</th>
<th>$\Omega_m$</th>
<th>$\Omega_{m,corr}$</th>
<th>$C_{\Omega,m,corr}$</th>
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<td>1</td>
<td>850</td>
<td>Ideal</td>
<td>Fickian</td>
<td>$1.26 \times 10^4$</td>
<td>$1.24 \times 10^4$</td>
<td>1.01386</td>
</tr>
<tr>
<td>2</td>
<td>Heptane-Air</td>
<td>1</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$7.76 \times 10^4$</td>
<td>$6.45 \times 10^4$</td>
<td>1.203619</td>
</tr>
<tr>
<td>3</td>
<td>Heptane-Oxygen</td>
<td>10</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$1.98 \times 10^4$</td>
<td>$1.64 \times 10^4$</td>
<td>12.1116</td>
</tr>
<tr>
<td>4</td>
<td>Heptane-Oxygen</td>
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<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$7.10 \times 10^5$</td>
<td>$6.41 \times 10^5$</td>
<td>11.0767</td>
</tr>
<tr>
<td>5</td>
<td>Heptane-Air</td>
<td>35</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$1.34 \times 10^5$</td>
<td>$5.59 \times 10^5$</td>
<td>23.8764</td>
</tr>
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<td>6</td>
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<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$7.10 \times 10^5$</td>
<td>$6.41 \times 10^5$</td>
<td>11.0767</td>
</tr>
<tr>
<td>7</td>
<td>Heptane-Air</td>
<td>100</td>
<td>850</td>
<td>Ideal</td>
<td>Fickian</td>
<td>$1.27 \times 10^5$</td>
<td>$1.03 \times 10^5$</td>
<td>0.12392</td>
</tr>
<tr>
<td>8</td>
<td>Heptane-Air</td>
<td>35</td>
<td>1300</td>
<td>Real</td>
<td>Generalized</td>
<td>$3.02 \times 10^5$</td>
<td>$2.75 \times 10^5$</td>
<td>10.9642</td>
</tr>
<tr>
<td>9</td>
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<td>100</td>
<td>1300</td>
<td>Real</td>
<td>Generalized</td>
<td>$4.70 \times 10^5$</td>
<td>$4.86 \times 10^5$</td>
<td>9.67441</td>
</tr>
</tbody>
</table>

Table 3.1: Comparison of calculated and corrected mixing frequencies ($\Omega_m$) for various test cases. All the test cases are for non-reacting (mixing) flows.
Table 3.2: Comparison of norm of residuals of CSD obtained from DNS and curve fit data from IECM model.

<table>
<thead>
<tr>
<th>Case</th>
<th>Species</th>
<th>$P_0$ (atm)</th>
<th>$Re$</th>
<th>EOS</th>
<th>Diffusion</th>
<th>Norm of Residual</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
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<tr>
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<td>Heptane-Air</td>
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<td>850</td>
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<td>Fickian</td>
<td>$4.4 \times 10^3$</td>
</tr>
<tr>
<td>2</td>
<td>Heptane-Air</td>
<td>1</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$2.75 \times 10^3$</td>
</tr>
<tr>
<td>3</td>
<td>Heptane-Oxygen</td>
<td>10</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$5.1 \times 10^3$</td>
</tr>
<tr>
<td>4</td>
<td>Heptane-Oxygen</td>
<td>100</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$2.5 \times 10^3$</td>
</tr>
<tr>
<td>5</td>
<td>Heptane-Air</td>
<td>35</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>$5.2 \times 10^3$</td>
</tr>
<tr>
<td>6</td>
<td>Heptane-Air</td>
<td>100</td>
<td>850</td>
<td>Ideal</td>
<td>Fickian</td>
<td>$6.9 \times 10^3$</td>
</tr>
<tr>
<td>7</td>
<td>Heptane-Air</td>
<td>100</td>
<td>1300</td>
<td>Real</td>
<td>Generalized</td>
<td>$5.1 \times 10^3$</td>
</tr>
<tr>
<td>8</td>
<td>Heptane-Air</td>
<td>35</td>
<td>1300</td>
<td>Real</td>
<td>Generalized</td>
<td>$5.2 \times 10^3$</td>
</tr>
<tr>
<td>9</td>
<td>Heptane-Air</td>
<td>100</td>
<td>1300</td>
<td>Ideal</td>
<td>Fickian</td>
<td>$6.9 \times 10^3$</td>
</tr>
</tbody>
</table>

Table 3.3: Modeling constants for the IEM, MC and MAPPING models for various test cases.

<table>
<thead>
<tr>
<th>Case</th>
<th>Species</th>
<th>$P_0$ (atm)</th>
<th>$Re$</th>
<th>EOS</th>
<th>Diffusion</th>
<th>$C_{IEM}$</th>
<th>$C_{MC}$</th>
<th>$C_{MAP}$</th>
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<tbody>
<tr>
<td>1</td>
<td>Heptane-Air</td>
<td>1</td>
<td>850</td>
<td>Ideal</td>
<td>Fickian</td>
<td>1</td>
<td>1</td>
<td>$-2 \times 10^{-2}$</td>
</tr>
<tr>
<td>2</td>
<td>Heptane-Air</td>
<td>1</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>1</td>
<td>2</td>
<td>$5 \times 10^{-2}$</td>
</tr>
<tr>
<td>3</td>
<td>Heptane-Oxygen</td>
<td>10</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>0.5</td>
<td>1</td>
<td>$9 \times 10^{-3}$</td>
</tr>
<tr>
<td>4</td>
<td>Heptane-Oxygen</td>
<td>100</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>0.75</td>
<td>1</td>
<td>$9.5 \times 10^{-3}$</td>
</tr>
<tr>
<td>5</td>
<td>Heptane-Air</td>
<td>35</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>0.75</td>
<td>1</td>
<td>$2 \times 10^{-2}$</td>
</tr>
<tr>
<td>6</td>
<td>Heptane-Air</td>
<td>100</td>
<td>850</td>
<td>Real</td>
<td>Generalized</td>
<td>1</td>
<td>1</td>
<td>$4 \times 10^{-2}$</td>
</tr>
<tr>
<td>7</td>
<td>Heptane-Air</td>
<td>100</td>
<td>850</td>
<td>Ideal</td>
<td>Fickian</td>
<td>1</td>
<td>1</td>
<td>$3 \times 10^{-3}$</td>
</tr>
<tr>
<td>8</td>
<td>Heptane-Air</td>
<td>35</td>
<td>1300</td>
<td>Real</td>
<td>Generalized</td>
<td>1</td>
<td>0.875</td>
<td>$2 \times 10^{-2}$</td>
</tr>
<tr>
<td>9</td>
<td>Heptane-Air</td>
<td>100</td>
<td>1300</td>
<td>Real</td>
<td>Generalized</td>
<td>1</td>
<td>1</td>
<td>$6 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 3.4: Model constants for mixing frequency obtained from mean turbulent kinetic energy and mean dissipation rates. $\tau$ and $\bar{k}$ calculated from DNS of mixing of heptane and oxygen.
Figure 3.1: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 1\text{atm}$, $Re_0 = 850$ with the generalized diffusion model. Data extracted at $x_1 = 24D_{\text{jet}}$.

Figure 3.2: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 35\text{atm}$, $Re_0 = 850$ with the generalized diffusion model. Data extracted at $x_1 = 24D_{\text{jet}}$. 
Figure 3.3: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 100$ atm, $Re_0 = 850$ with the generalized diffusion model. Data extracted at $x = 24D_{jet}$.

Figure 3.4: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 1$ atm, $Re_0 = 1300$ with the generalized diffusion model. Data extracted at $x = 24D_{jet}$. 
Figure 3.5: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 35\text{atm}$, $Re_0 = 1300$ with the generalized diffusion model. Data extracted at $x_1 = 24D_{jet}$.

Figure 3.6: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 100\text{atm}$, $Re_0 = 1300$ with the generalized diffusion model. Data extracted at $x_1 = 24D_{jet}$.
Figure 3.7: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 1$ atm, $Re_0 = 850$ with the standard Fickian diffusion model. Data extracted at $x_1 = 24D_{jet}$.

Figure 3.8: Filtered mass density function of mixture fraction measured from DNS at $P_0 = 100$ atm, $Re_0 = 850$ with the standard Fickian diffusion model. Data extracted at $x_1 = 24D_{jet}$. 
Figure 3.9: Conditional Scalar Diffusion measured from DNS at \( P_0 = 1 \text{atm}, \ Re_0 = 850 \) with the generalized diffusion model at times \( t^* = 75, 150, 190 \). Data extracted along the jet centerline at \( x_1 = 15D_{jet} \).

Figure 3.10: Conditional Scalar Diffusion measured from DNS at \( P_0 = 35 \text{atm}, \ Re_0 = 850 \) with the generalized diffusion model at times \( t^* = 75, 150, 190 \). Data extracted along the jet centerline at \( x_1 = 15D_{jet} \).
Figure 3.11: Conditional Scalar Diffusion measured from DNS at $P_0 = 100\text{atm}$, $Re_0 = 850$ with the generalized diffusion model at times $t^* = 75, 150, 190$. Data extracted along the jet centerline at $x_1 = 15D_{\text{jet}}$.

Figure 3.12: Conditional Scalar Diffusion measured from DNS at $P_0 = 1\text{atm}$, $Re_0 = 1300$ with the generalized diffusion model at times $t^* = 75, 150, 190$. Data extracted along the jet centerline at $x_1 = 15D_{\text{jet}}$. 
Figure 3.13: Conditional Scalar Diffusion measured from DNS at $P_0 = 35\text{atm}$, $Re_0 = 1300$ with the generalized diffusion model at times $t^* = 75, 150, 190$. Data extracted along the jet centerline at $x_1 = 15D_{jet}$.

Figure 3.14: Conditional Scalar Diffusion measured from DNS at $P_0 = 100\text{atm}$, $Re_0 = 1300$ with the generalized diffusion model at times $t^* = 75, 150, 190$. Data extracted along the jet centerline at $x_1 = 15D_{jet}$.
Figure 3.15: Conditional Scalar Diffusion measured from DNS at $P_0 = 1\text{atm}$, $Re_0 = 850$ with the Fickian diffusion model at times $t^* = 75, 150, 190$. Data extracted along the jet centerline at $x_1 = 15D_{jet}$.

Figure 3.16: Conditional Scalar Diffusion measured from DNS at $P_0 = 100\text{atm}$, $Re_0 = 850$ with the Fickian diffusion model at times $t^* = 75, 150, 190$. Data extracted along the jet centerline at $x_1 = 15D_{jet}$.
Figure 3.17: Conditional average of arbitrary function \( f \) modeled by the IEM/LMSE model.
Figure 3.18: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 1$ atm, $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model. $\Omega_{m, calculated} = 1.26 \times 10^4$. 
\( \Omega_{m,\text{calculated}} = -7.76 \times 10^3 \)

\( \Omega_{m,\text{corrected}} = 6.45 \times 10^3 \)

Figure 3.19: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at \( P_0 = 1\text{atm}, \quad Re_0 = 850 \) with real gas equation of state and the generalized diffusion model.
Figure 3.20: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-oxygen mixture at $P_0 = 10\text{ atm}$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.

(a) $\Omega_{m,\text{calculated}} = 1.95 \times 10^5$

(b) $\Omega_{m,\text{corrected}} = 1.64 \times 10^4$
Figure 3.21: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-oxygen mixture at $P_0 = 100\ atm$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.

(a) $\Omega_{m,\text{calculated}} = 7.10 \times 10^6$

(b) $\Omega_{m,\text{corrected}} = 6.41 \times 10^5$
Figure 3.22: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 35\, atm$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.
Figure 3.23: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\text{ atm}$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.

(a) $\Omega_{m,\text{calculated}} = 7.10 \times 10^6$

(b) $\Omega_{m,\text{corrected}} = 6.41 \times 10^5$
Figure 3.24: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 100$ atm, $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model.
Figure 3.25: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 1\text{atm}$, $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model.
Figure 3.26: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 35\text{atm}$, $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model.

(a) $\Omega_{m,calculated} = 3.02 \times 10^6$

(b) $\Omega_{m,corrected} = 2.75 \times 10^5$
Figure 3.27: CSD modeled by the IEM, MC and MAPPING models. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\text{atm}$, $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model.
Figure 3.28: CSD modeled by the IECM model. CSD obtained from DNS of heptane-air mixture at $P_0 = 1\text{ atm}$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model. The mixing frequency for this model is same as that of the IEM model.

Figure 3.29: CSD modeled by the IECM model. CSD obtained from DNS of heptane-air mixture at $P_0 = 1\text{ atm}$, $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model. The mixing frequency for this model is same as that of the IEM model.
Figure 3.30: CSD modeled by the IECM model. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\text{ atm}$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model. The mixing frequency for this model is same as that of the IEM model.

Figure 3.31: CSD modeled by the IECM model. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\text{ atm}$, $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model. The mixing frequency for this model is same as that of the IEM model.
Figure 3.32: CSD modeled by the IECM model. CSD obtained from DNS of heptane-air mixture at $P_0 = 1\, atm$, $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model. The mixing frequency for this model is same as that of the IEM model.

Figure 3.33: CSD modeled by the IECM model. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\, atm$, $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model. The mixing frequency for this model is same as that of the IEM model.
Figure 3.34: CSD modeled by the MAPPING model. The scalar value in the model remains unsorted. CSD obtained from DNS of heptane-air mixture at $P_0 = 1\text{ atm}$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.

Figure 3.35: CSD modeled by the MAPPING model. The scalar value in the model remains unsorted. CSD obtained from DNS of heptane-air mixture at $P_0 = 1\text{ atm}$, $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model.
Figure 3.36: CSD modeled by the MAPPING model. The scalar value in the model remains unsorted. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\text{atm}$, $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.

Figure 3.37: CSD modeled by the MAPPING model. The scalar value in the model remains unsorted. CSD obtained from DNS of heptane-air mixture at $P_0 = 100\text{atm}$, $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model.
Figure 3.38: Variation of calculated mixing frequency with ambient pressure. $\Omega_{m,\text{calc}}$ for flow at $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model.

Figure 3.39: Variation of parameters of mixing frequency with ambient pressure. $\langle \rho \rangle$, $\gamma_{\text{dev}}$, $\Delta_2^2$, $\sqrt{\xi}$ from flow at $Re_0 = 850$ with ideal gas equation of state and the Fickian diffusion model.
Figure 3.40: Variation of calculated mixing frequency with ambient pressure. $\Omega_{m,\text{calc}}$ for flow at $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.

Figure 3.41: Variation of parameters of mixing frequency with ambient pressure. $\langle \rho \rangle_t$, $\gamma_{\text{dev}}$, $\Delta^2_G$, $\sqrt{\xi}$ from flow at $Re_0 = 850$ with real gas equation of state and the generalized diffusion model.
Figure 3.42: Variation of calculated mixing frequency with ambient pressure. $\Omega_m, \text{calc}$ for flow at $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model.

Figure 3.43: Variation of parameters of mixing frequency with ambient pressure. $\langle \rho \rangle_t, \gamma_{\text{dev}}, \Delta G^2, \sqrt{\xi}$ from flow at $Re_0 = 1300$ with real gas equation of state and the generalized diffusion model.
Figure 3.44: Comparison of conditionally averaged mixing frequency and conditionally averaged second invariant of strain tensor, $II(s_{ij})$ calculated from DNS at $P_0 = 1\text{ atm}, Re_0 = 850$ with the generalized diffusion model.

Figure 3.45: Comparison of conditionally averaged mixing frequency and conditionally averaged second invariant of strain tensor, $II(s_{ij})$ calculated from DNS at $P_0 = 35\text{ atm}, Re_0 = 850$ with the generalized diffusion model.
Figure 3.46: Comparison of conditionally averaged mixing frequency and conditionally averaged second invariant of strain tensor. $I(s_{ij})$ calculated from DNS at $P_0 = 100$ atm, $Re_0 = 850$ with the generalized diffusion model.
Chapter 4

RANS Budget Analysis

In RANS, the time averaged equations of motion are solved. As a result only the mean flow properties are captured and the effects of turbulence at all scales are modeled. The advantage of the RANS method is that it is computationally efficient and can be fairly accurate even for complex flows. However, since all the length scales of turbulence are modeled, care must be taken while applying RANS method to turbulent flows. It’s the most widely used approach in commercial CFD codes. The accuracy of RANS in turbulent flows depends upon the type of flow and the model used. A few modeling approaches will be discussed briefly in this section.

4.1 RANS Governing Equations

Reynolds decomposition is applied to all the flow variables in the governing equations and the instantaneous flow quantities are decomposed into time averaged and fluctuating components.

\[
\overline{\phi}(x, t) = \frac{1}{\tau} \int_{t}^{t+\tau} \phi(x', t')dt',
\]

where \( \tau \) represents the prescribed constant time interval, \( \overline{\phi} \) represents the time average of the instantaneous quantity \( \phi \) and \( \phi' \) represents the fluctuation about the mean. A few important rules are
applicable to Reynolds decomposition which enable reduction of terms in the governing equations:

\[
\begin{align*}
\bar{\phi} &= \bar{\phi}, \\
\bar{\phi}' &= 0, \\
\bar{\phi}_1 + \bar{\phi}_2 &= \bar{\phi}_1 + \bar{\phi}_2, \\
\bar{\phi}_1 \bar{\phi}_2 &= \bar{\phi}_1 \bar{\phi}_2, \\
\bar{\phi}_1 \bar{\phi}_2 &= 0, \\
\bar{\phi}_1 \bar{\phi}_2 &= \bar{\phi}_1 \bar{\phi}_2 + \bar{\phi}'_1 \bar{\phi}'_2.
\end{align*}
\] (4.2)

These rules, when applied to the incompressible Navier Stokes equations, directly result in the RANS governing equations. However, in compressible flows, application of these rules result in a number of non-zero terms. Thus, a density weighted averaging method called Favre averaging is applied to the compressible equations. The Favre average of a quantity \( \phi \) is given as,

\[
\tilde{\phi} = \rho \bar{\phi}/\bar{\rho}, \\
\bar{\rho} \bar{\phi} = \bar{\rho} \tilde{\phi}, \\
\phi = \bar{\phi} + \phi''.
\] (4.3)

Similar to Reynolds decomposition a few rules are applicable to Favre averaging which enable reduction of terms in the governing equations.

\[
\begin{align*}
\bar{\phi}'' &\neq 0, \\
\bar{\rho} \bar{\phi}'' &= 0, \\
\bar{\rho} \phi_1 \phi_2 &= \bar{\rho} \tilde{\phi}_1 \tilde{\phi}_2 + \bar{\rho} \phi''_1 \phi''_2.
\end{align*}
\] (4.4)

The instantaneous flow variables of compressible equations are decomposed as,

\[
\begin{align*}
\rho &= \bar{\rho} + \rho', \\
\bar{u}_i &= \bar{u}_i + u''_i, \\
p &= \bar{p} + p', \\
\bar{e}_t &= \bar{e}_t + e''_t.
\end{align*}
\] (4.5)
Application of this decomposition to Eqs.(2.1-2.4) results in a new set of equations applicable to RANS for compressible flows.

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} [\rho \tilde{u}_j] = 0, \quad (4.6)
\]

\[
\frac{\partial}{\partial t} (\rho \tilde{u}_i) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_i \tilde{u}_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} [\tau_{ij} - \rho u_i' u_j'], \quad (4.7)
\]

\[
\frac{\partial}{\partial t} (\rho \tilde{e}_t) + \frac{\partial}{\partial x_j} [(\rho \tilde{e}_t + P) \tilde{u}_j] = \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \tau_{ij} + u_i' \tau_{ij} - Pu_j' \right] - \frac{\partial}{\partial x_j} (\rho \tilde{e}_t \tilde{u}_j) + \frac{\partial}{\partial x_j} \left[ \sum_\beta H_i^\beta \tilde{J}_i^\beta \right], \quad (4.8)
\]

\[
\frac{\partial}{\partial t} (\rho \tilde{Y}_\beta) + \frac{\partial}{\partial x_j} (\rho \tilde{Y}_\beta \tilde{u}_j) = \frac{\partial}{\partial x_j} (\tilde{J}_j^\beta) - \frac{\partial}{\partial x_j} (\rho \tilde{Y}_\beta \tilde{u}_j) \quad (4.9)
\]

with

\[
\tau_{ij} = \mu \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right), \quad (4.10)
\]

and,

\[
\bar{P} = \frac{R T}{\tau - B_m} - \frac{A_m}{\tau^2 + 2\pi B_m - B_m^2}. \quad (4.11)
\]

In the momentum equation, the term \(\rho u_i' u_j'\) represents the Reynolds stress tensor:

\[
R_{ij} = u_i' u_j' = \frac{\rho u_i' u_j'}{\rho}. \quad (4.12)
\]

\(R_{ij}\) represents the source of turbulence in RANS. The terms of similar form in the energy equation \((\rho e_t' u_j')\) and species transport equation \((\rho Y' u_j')\) are called turbulent energy flux and turbulent mass flux, respectively. These terms remain unclosed in the governing equations and require modeling. A number of models have been proposed to close these terms and in the process capture the effects of turbulence. The modeling approaches may be broadly classified into the following categories, i) Linear eddy viscosity models, ii) Non-linear eddy viscosity models and iii) Reynolds stress models.

In the linear eddy viscosity models, the Reynolds stress tensor is modeled using the Boussinesq’s hypothesis [105] which prescribes a linear constitutive relationship between \(R_{ij}\) and the mean
strain rate tensor ($\sigma_{ij}$):

$$-pR_{ij} = 2\mu_t \left( \frac{1}{3} \frac{\partial \tilde{u}_i}{\partial x_j} \delta_{ij} \right) - \frac{2}{3} p k \delta_{ij},$$

$$\sigma_{ij} = \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i},$$

(4.13)

where $\mu_t = C \bar{p} k^2 / \epsilon$ represents the turbulence eddy viscosity, $k$ the turbulence kinetic energy and $\epsilon$ the turbulence dissipation rate. The zero equation models (algebraic models), one-equation models and two-equation models are classified as linear eddy viscosity models. These models attempt to resolve the turbulence eddy viscosity term from the flow using empirical relationships or through solution of transport equations for the turbulence kinetic energy and turbulence dissipation rate. In non-linear eddy viscosity models $R_{ij}$ is related to $(\sigma_{ij})$ and mean rotation tensor $(\Omega_{ij})$ through a non-linear relationship. The reader is referred to the works of Yang and Ma [106] and Craft [107, 108] for detailed discussions on linear and non-linear eddy viscosity models.

The third class of models called the Reynolds stress models (RSM) are typically second or higher order turbulence closure models. In these models, a transport equation for the Reynolds stress tensor is derived to obtain various terms that physically represent production, diffusion, dissipation and transport of turbulence in the flow. These terms are either directly resolved or modeled to account for complex interactions within the flow field. These models avoid the simplifications used in eddy viscosity models and so among RANS models, RSM captures the most effects of turbulence.

In this work the RSM is presented only for the Reynolds stress tensor in the momentum equation. A similar approach may be employed to obtain the transport equations and models for turbulent energy flux and mass flux terms. The following identity is employed to derive the transport equation for the Reynolds stress,

$$\frac{\partial}{\partial t} \rho \tilde{u}_i \tilde{u}_j'' = \frac{\partial}{\partial t} \rho \tilde{u}_i \tilde{u}_j - \frac{\partial}{\partial t} \rho \tilde{u}_i \tilde{u}_j.$$

(4.14)

The two terms on the right hand side in the above equation may be obtained using the following identities,

$$\frac{\partial}{\partial t} \rho \tilde{u}_i \tilde{u}_j = \frac{\partial}{\partial t} \rho \tilde{u}_i \tilde{u}_j = \tilde{u}_j \left( \frac{\partial \rho \tilde{u}_i}{\partial t} \right) + \tilde{u}_i \left( \rho \frac{\partial \tilde{u}_j}{\partial t} \right),$$

(4.15)

$$\frac{\partial}{\partial t} \rho \tilde{u}_i \tilde{u}_j' = \tilde{u}_j \left( \frac{\partial \rho \tilde{u}_i}{\partial t} \right) + \tilde{u}_i \left( \rho \frac{\partial \tilde{u}_j}{\partial t} \right).$$

(4.16)
The first and second terms on the right hand side of Eq.(4.15) represent the Reynolds average of product of velocity and conservative and non-conservative forms of momentum equation. The terms on the right hand side of Eq.(4.16) represent the product of Favre averaged velocity and the conservative and non-conservative forms of RANS momentum equation. The non-conservative form equations may be obtained from the conservative form of momentum equations by applying the continuity identity. The left hand side of the conservative form of momentum equation may be written as,

$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j),$$

(4.17)

and the left hand side of the non-conservative form of equation may be obtained from the above as,

$$\rho \frac{\partial u_i}{\partial t} + u_j \frac{\partial \rho}{\partial t} + \rho u_j \frac{\partial u_i}{\partial x_j} + \rho u_j \frac{\partial u_i}{\partial x_j},$$

(4.18)

The final form of transport equation for the Reynolds stress is obtained by application of all of the above identities to the RANS momentum equation. Alternatively this equation may be referred to as the Reynolds stress budget equation.

$$\frac{\partial}{\partial t} \rho u_i \overline{u_j} + \frac{\partial}{\partial x_k} \rho u_i \overline{u_j} \overline{u_k} = \frac{\partial}{\partial x_k} \left[ -\rho u_i u_j u_k - \rho u_i u_j \delta_{ik} - \rho \overline{u_i u_j} \delta_{ik} + \overline{u_i u_j} \delta_{ik} + \overline{u_i u_j} \delta_{ik} + \overline{u_i u_j} \delta_{ik} \right]$$

$$+ \rho \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left( -\rho u_i u_j \frac{\partial \overline{u_j}}{\partial x_i} - \rho u_j \frac{\partial \overline{u_i}}{\partial x_j} \right) - \left( \tau_i \frac{\partial \overline{u_j}}{\partial x_k} + \tau_j \frac{\partial \overline{u_i}}{\partial x_k} \right)$$

$$+ \left( -u_i \frac{\partial \overline{P}}{\partial x_j} - u_j \frac{\partial \overline{P}}{\partial x_i} + u_i \frac{\partial \overline{\tau_i}}{\partial x_k} + u_j \frac{\partial \overline{\tau_j}}{\partial x_k} \right).$$

(4.19)

This equation may be re-written in terms of $R_{ij}$ as,

$$\frac{\partial}{\partial t} \rho R_{ij} + \frac{\partial}{\partial x_k} \rho R_{ij} \overline{u_k} = \frac{\partial}{\partial x_k} \left[ -\rho u_i u_j u_k - \rho u_i u_j \delta_{ik} - \rho \overline{u_i u_j} \delta_{ik} + \overline{u_i u_j} \delta_{ik} + \overline{u_i u_j} \delta_{ik} + \overline{u_i u_j} \delta_{ik} \right]$$

$$+ \rho \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) + \left( -\rho R_{ik} \frac{\partial \overline{u_j}}{\partial x_i} - \rho R_{jk} \frac{\partial \overline{u_i}}{\partial x_k} \right) - \left( \tau_i \frac{\partial \overline{u_j}}{\partial x_k} + \tau_j \frac{\partial \overline{u_i}}{\partial x_k} \right)$$

$$+ \left( -u_i \frac{\partial \overline{P}}{\partial x_j} - u_j \frac{\partial \overline{P}}{\partial x_i} + u_i \frac{\partial \overline{\tau_i}}{\partial x_k} + u_j \frac{\partial \overline{\tau_j}}{\partial x_k} \right).$$

(4.20)

$$\text{convection (C)}$$

$$\text{diffusion (D)}$$

$$\text{pressure-strain (P)}$$

$$\text{production (P)}$$

$$\text{dissipation (e)}$$

$$\text{density-fluctuation effects (\zeta)}$$
This budget equation accounts for all the physical processes (convection, diffusion, production, dissipation and strain) that dictate the transport of $R_{ij}$ and the solution of this equation results in resolution of effects of turbulence.

4.2 Reynolds Stress Budget Measurement

In traditional RANS simulations with RSM models, the Reynolds stress transport equation is solved with appropriate models for various terms [in Eq.(4.20)] to resolve $R_{ij}$. However, accuracy of this solution largely depends upon the models chosen for various terms in the budget equation. In this work, all the terms of the Reynolds stress budget equation are directly measured from the DNS and compared against various models to study the applicability of the models in shear flows over a large range of pressures. Measurement of the budget terms from the DNS is performed in three stages.

1. The DNS is run until a statistically stationary state of the flow is achieved. A turbulent flow is said to reach a statistically stationary state when statistics of the flow (mean, variance) become invariant with time. This time instant will be referred to as $t_{\text{begin}}$. The simulation is then advanced for a prescribed length of time ($\Delta t_s$). This instant will be referred to as $t_{\text{end1}} = t_{\text{begin}} + \Delta t_s$. At this point the properties of the flow ($\rho, u_i, P, \mu$) are stored into an output file. The Reynolds average of flow properties ($\bar{\rho}, \bar{u}_i, \bar{P}, \bar{\mu}$) are also calculated at this instant. These averages are then stored into a separate file.

2. The simulation is restarted again at $t_{\text{begin}}$ with stored averages of flow properties and the instantaneous fluctuations in flow properties ($\rho', u'_i, P', \mu'$) and the Reynolds stress terms ($\rho u'_i u'_j$) are calculated. The simulation is then run until a statistically stationary state of fluctuating components is achieved. This time instant will be referred to as $t_{\text{end2}}$. At this instant, the Reynolds average of the fluctuating components ($\bar{\rho} u'_i u'_j, \bar{u}'_i$) are calculated and stored into a separate file.

3. In the final stage instantaneous values of the individual budget terms are calculated and the simulation is advanced until a statistically stationary state of budget terms is achieved. At this instant, the Reynolds average of individual budget terms are calculated.
The budget terms are calculated throughout the domain to obtain spatial variations at various locations within the flow. The statistically stationary state of the budget terms implies temporal invariance of the Reynolds stress tensor,

$$\frac{\partial}{\partial t} \rho \overline{R_{ij}} = 0,$$

$$\Rightarrow C_{ij} = \frac{\partial}{\partial x_k} \rho \overline{R_{ij} u_k''}$$

Thus, Eq.(4.20) may be re-written as,

$$\frac{\partial}{\partial x_k} \rho R_{ij} \tilde{u}_k'' = \beta_{ij},$$

(4.22)

where $\beta_{ij} = D_{ij} + \Pi_{ij} + P_{ij} + \epsilon_{ij} + \zeta_{ij}$ represents the sum of diffusion, pressure-strain, production, dissipation and density fluctuation effects. The budget of $R_{ij}$ measured across the slot jets at the center of the domain is presented in Figs. 4.1-4.5. The terms are measured at each grid point in the DNS domain and, as a result, the trends of the budget terms are multi-modal. It is observed that the diffusion and pressure-strain terms have significantly larger magnitudes than the other terms. In Eq.(4.20), the convection ($C_{ij}$) and production terms ($P_{ij}$) are exact and require no modeling. However, the diffusion ($D_{ij}$), pressure-strain ($\Pi_{ij}$), dissipation ($\epsilon_{ij}$) and density-fluctuation ($\zeta_{ij}$) terms require modeling.

The balance of $C_{ij}$ and $\beta_{ij}$ is presented in Figs. 4.6-4.10. At some instances, a slight difference between the two terms is observed ($|C_{ij} - \beta_{ij}| > 0$). In theory this difference can be corrected by averaging over very long simulation run times. However, in simulations the artificial turbulence forcing methods get dampened over a period of time and the simulations are prone to numerical diffusion over lengthy runs.

### 4.3 Modeling of Budget Terms

In previous attempts of modeling turbulence using RSM, the effects of ambient pressure on turbulence and its implications on the models have been overlooked. This work evaluates several different models for the budget terms in the Reynolds stress transport equation at various ambient pressures and proposes appropriate modifications to the existing models. Least-squares curve fitting method is applied and the modeling constants are calibrated to fit the data obtained from DNS.
Ratio of norms of residuals (for a linear curve fit) of the DNS data and models (with unity model constant values) are calculated for each component of the tensor. An average value (of ratios of norms of residuals) is then determined such that a single model constant can be applied to all the components of the tensor for the best curve fit.

4.3.1 Compressibility Term

The effect of compressibility is usually neglected in many shear flows and wall bounded flows. This term is considered to be significant only in supersonic flows or in reacting flows at high pressures and large Mach numbers. Development of a model for this term would require extensive validation of a baseline model over a large range of Mach numbers [109]. Models for compressibility terms have been proposed by Livescu and Ristorcelli [110] and Ristorcelli [111]. In this study (mixing flow, \( Ma_c = 0.35 \)), the magnitude of \( \zeta_{ij} \) is observed to be significantly smaller than all the other terms. The balance of \( C_{ij} \) with \( \beta_{ij} - \zeta_{ij} \) is presented in Figs. 4.11-4.15. It is observed that there is no change in trend or magnitude of \( \beta_{ij} \) when the compressibility term is omitted, even at high pressures.

4.3.2 Diffusion Term

The diffusion term \( (D_{ij}) \) has been modeled by a number of different approaches. Most of the models are based on the traditional turbulent eddy diffusivity approach used in eddy viscosity models. The diffusion term is split as turbulent diffusion term and molecular diffusion term.

\[
D_{ij} = \frac{\partial}{\partial x_k} \left[ -P' u_i'' u_j'' \right] + \frac{\partial}{\partial x_k} \left[ P' u_i'' \delta_{ik} - P' u_i'' \delta_{jk} + u_i'' \tau_{kj} + u_j'' \tau_{ki} \right].
\] (4.23)

The molecular diffusion term can be further decomposed as,

\[
D_{ij}^m = \frac{\partial}{\partial x_k} \left( P' u_j'' \delta_{ik} - P' u_i'' \delta_{jk} \right) + \frac{\partial}{\partial x_k} \left( u_i'' \tau_{kj} + u_j'' \tau_{ki} \right),
\] (4.24)

where the first term on the right hand side of the equation indicates the contribution from pressure diffusion \( (D_{ij}^p) \) and the second term indicates contribution from viscous diffusion \( (D_{ij}^v) \). Some of the most widely used models are evaluated and discussed in this section.
4.3.2.1 Molecular Diffusion Models

In the model proposed by Lien and Leschziner [112], the molecular diffusion term is modeled as,

\[ D_{ij}^m = \frac{\partial}{\partial x_k} \left[ \bar{\mu} \frac{\partial R_{ij}}{\partial x_k} \right]. \tag{4.25} \]

In Daly and Harlow [113], Mellor and Herring [114] and Hanjalic and Launder [115] models this term is modeled as,

\[ D_{ij}^m = \frac{\partial T_{ijk}^m}{\partial x_k} = C_m \frac{\partial}{\partial x_k} \left[ \bar{\mu} \left( \frac{\partial R_{jk}}{\partial x_i} + \frac{\partial R_{ki}}{\partial x_j} + \frac{\partial R_{ij}}{\partial x_k} \right) \right], \tag{4.26} \]

with \( C_m = 1 \). In the above equations, \( \bar{\mu} \) represents the mean viscosity.

4.3.2.2 Turbulent Diffusion Models

In the aforementioned models, the triple correlations (\( T_{ijk}^t = u_i'' u_j'' u_k'' \)) in the turbulent diffusion term (\( D_{ij}^t = \frac{\partial T_{ijk}^t}{\partial x_k} \)) are modeled using the following models:

- Lien and Leschziner model

\[ T_{ijk}^t = \bar{p} \mu_t \frac{\partial R_{ij}}{\sigma_k \partial x_k} \tag{4.27} \]

where \( \mu_t = C_{\mu} \bar{p} k^2 / \epsilon \) represents the turbulent eddy viscosity, \( C_{\mu} \) the model constant and \( \sigma_k \) is an adjustable constant. For the base model evaluation, the values of model constants used were, \( C_{\mu} = 0.09 \), and \( \sigma_k = 0.81 \).

- Mellor and Herring model

\[ T_{ijk}^t = \bar{p} C_t \frac{k^2}{\epsilon} \left( \frac{\partial R_{jk}}{\partial x_i} + \frac{\partial R_{ki}}{\partial x_j} + \frac{\partial R_{ij}}{\partial x_k} \right), \tag{4.28} \]

with \( C_t = 0.11 \).

- Daly and Harlow model

\[ T_{ijk}^t = \bar{p} C_t \frac{k}{\epsilon} R_{ij} \frac{\partial R_{ij}}{\partial x_i}, \tag{4.29} \]

with \( C_t = 0.22 \).
Hanjalic and Launder model

\[ T_{ijk}^t = \bar{p}C_t \frac{k}{\epsilon} \left( R_{il} \frac{\partial R_{jk}}{\partial x_l} + R_{jl} \frac{\partial R_{ki}}{\partial x_l} + R_{kl} \frac{\partial R_{ij}}{\partial x_l} \right), \]  

(4.30)

with \( C_t = 0.11 \).

In Eqs.(4.26-4.30), \( C_m \) and \( C_t \) represent the model constants for molecular and turbulent diffusion, respectively. \( C_t \) is similar in form to the ratio \( C_\mu/\sigma_k \) in the Lien and Leschziner model. Among the turbulent diffusion models, the Lien and Leschziner model and the Mellor and Herring model are linear in \( R_{ij} \) and as a result do not exhibit tensorial symmetry [116]. However, only 10 components of the tensor are presented in Figs. 4.21-4.25. The Daly and Harlow model is simple in its form but has been shown to not adequately describe the triple velocity correlations \( T_{ijk}^t = u_i' u_j' u_k' \) in the works of Kurbatskii and Poroseva [117]. The Hanjalic and Launder model is more complex but preserves the tensorial symmetry of \( T_{ijk}^t \). Although the predictions of this model are less accurate than models based on transport equation of \( T_{ijk}^t \), the results are shown to be comparable in the works of Poroseva [118].

In this work, the molecular diffusion and triple velocity moments are calculated directly from DNS and compared against the models. Values of model constants \( C_\mu, \sigma_k, C_m \) and \( C_t \) as a function of pressure are proposed in the Section (4.4). The accuracy of all the models depend on turbulent kinetic energy and diffusion rates. This would require solutions of additional transport equations for \( k \) and \( \epsilon \). In this work, the turbulence kinetic energy \( (k = \frac{1}{2} [R_{11} + R_{22} + R_{33}] ) \) and the turbulence dissipation rate \( (\epsilon = \frac{1}{2} [\epsilon_{11} + \epsilon_{22} + \epsilon_{33}] ) \) are directly computed from the DNS. The trends of triple velocity correlations (turbulent diffusion) are presented in Figs. 4.26-4.30. The data from the Lien and Leschziner model considering the combined effect of molecular and turbulent diffusion is presented in Figs. 4.16-4.20. It is observed that all the models predict trends that are qualitatively similar to the triple velocity moments. At many instances the models also fit exactly or over/under-predict the DNS data. The Mellor and Herring model is observed to be under-predicting the DNS data while the Daly and Harlow model and the Hanjalic and Launder model tend to over-predict.

In modeling of triple velocity moments, a slightly over-predictive model could prove to be better for engineering applications and account as factor of safety. The model constant \( C_t \) can further be tuned to obtain a better fit.
4.3.3 Pressure Strain Term

The pressure strain term redistributes the energy produced by shear into other components of the budget thereby reducing the anisotropy in shear flows. The anisotropic part transports the mean momentum in the Reynolds stress tensor. Modeling of pressure strain has been recognized as one of the more difficult tasks because the physical process is complex and involves parts of various transport mechanisms (production, dissipation, pressure dilation). The pressure strain term can be decomposed into slow strain, rapid strain and a wall term.

\[
\Pi_{ij} = \Pi_{ij}^s + \Pi_{ij}^r + \Pi_{ij}^w,
\]

where \(\Pi_{ij}^s\) represents the slow pressure strain term responsible for return to isotropic turbulence, \(\Pi_{ij}^r\) represents the rapid pressure strain term that responds directly to the mean velocity gradient and \(\Pi_{ij}^w\) represents the effects of wall on strain [119]. The models proposed for pressure strain are generally applicable only to specific types of flows. In this section, some of the modeling approaches are discussed.

4.3.3.1 Models for Incompressible Flows

One of the most popular models for pressure strain applicable to incompressible flows was proposed by Launder, Reece and Rodi (LRR) [120]. In this model, the slow and rapid terms are modeled as a linear function of the anisotropy tensor and the wall effects are neglected. A general form of the model may be written as,

\[
\Pi_{ij} = -C_1\bar{\rho}\tau_{ij} + C_1^'\bar{\rho}\epsilon \left( b_{ik}b_{kj} - \frac{1}{3}b_{mn}b_{mn}\delta_{ij} \right) \quad \text{slow part}
\]

\[
+ C_2\bar{\rho}k\bar{\omega}_{ij} + C_3\bar{\rho}k \left( b_{ik}\bar{\omega}_{jk} + b_{jk}\bar{\omega}_{ik} - \frac{2}{3}b_{mn}\bar{\omega}_{mn}\delta_{ij} \right) + C_4\bar{\rho}k \left( b_{ik}\Omega_{jk} + b_{jk}\Omega_{ik} \right) \quad \text{rapid part}
\]

where \(C_1, C_1', C_2, C_3, C_4\) are the model constants. The anisotropy tensor can be written as,

\[
b_{ij} = \left( \frac{\tau_{ij}}{2k} - \frac{1}{3}\delta_{ij} \right),
\]

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and the strain and rotation components can be written as,

\[ s_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij}, \]

\[ \Omega_{ij} = \frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} - \frac{\partial \tilde{u}_j}{\partial x_i} \right). \]  

(4.34)

Modifications to the LRR model was made by Gibson and Launder (GL) [121], to take into account wall effects. This model uses a quadratic formulation for the slow part and wall strain terms. For this study, there are no wall effects and the modified slow strain part is accounted for using a different value of model constant with the same general form of the pressure strain model as in Eq.(4.32).

The Speziale, Sarkar and Gatski (SSG) model [122] uses a form similar to the LRR model but with modified coefficients that take into account the effects of production, dissipation and anisotropy.

The standard model constants used for base model evaluation are [123],

- Launder, Reece and Rodi model

\[ C_1 = 3.0, C_2 = 0.8, C_3 = 1.75, C_4 = 1.31, C'_1 = 0, \]

(4.35)

- Gibson and Launder model

\[ C_1 = 3.6, C_2 = 0.8, C_3 = 1.2, C_4 = 1.2, C'_1 = 0, \]

(4.36)

- Speziale, Sarkar and Gatski model

\[ C_1 = 3.4 + 1.8(P_{ij}/\epsilon_{ij}), C_2 = 0.8 - 1.3(b_{ij}b_{ij})^{1/2}, \]

\[ C_3 = 1.25, C_4 = 0.4, C'_1 = 0. \]

(4.37)

The modified model constants as a function of pressure will be presented in the Section (4.4).

4.3.3.2 Models for Compressible Flows

The LRR model for incompressible flows was modified by Adumitroaei et al. [124] by considering non-zero divergence and pressure dilation effects to account for compressibility. Other modifications to the base model were proposed by Cambon et al. [125] that take into account the
variation of pressure strain due to Mach number. A physics based model for compressibility effects was proposed by Gomez and Girimaji (GG) [126]. This model takes into account the effects of pressure at different Mach number regimes. At high Mach numbers ($Ma_c >> 1$), the effects of pressure are said to be insignificant, at low Mach numbers ($Ma_c << 1$) the pressure acts rapidly to prevent any change in the divergence of velocity and at intermediate Mach numbers ($Ma_c \approx 1$) the pressure field causes a large amount of the flow thermodynamic interactions. The general form of this model may be written as,

$$\Pi_{ij} = -C_1 \rho \epsilon_{bi,j} + C_2 \rho k s_{i,j} + C_3 \rho k \left( b_{ik} s_{jk} + b_{jk} s_{ik} - \frac{2}{3} b_{mn} s_{mn} \delta_{ij} \right) + C_4 \rho k \left( b_{ik} \Omega_{jk} + b_{jk} \Omega_{ik} \right) - C_P \rho P_{ij}. \quad (4.38)$$

In this expression, $C_P$ is a function of the gradient Mach number. This model has a form similar to LRR model but has additional term to account for compressibility effects. The default values of model constants used for the baseline model evaluation are $C_1 = 3, C_2 = 0.8, C_3 = 1.75, C_4 = 1.31, C_P = 0.02$. The pressure strain models with variable parameters compared against ($\Pi_{ij}$) obtained from the DNS and are presented in Figs. 4.31-4.35.

### 4.3.4 Dissipation Term

The dissipation term is generally modeled by an isotropic tensor,

$$\Pi_{ij} = \frac{2}{3} \rho \delta_{ij} \epsilon, \quad (4.39)$$

where $\epsilon$ represents the isotropic tensor obtained from solution of additional transport equation for dissipation. The deviatoric terms are assumed to be covered by pressure-strain model. In this study the isotropic dissipation tensor is calculated directly from the DNS. The dissipation term obtained from DNS and that calculated from the model is presented in Figs. 4.36-4.40. It is observed that the closure for $\epsilon_{ij} \delta_{ij}$ is accurate. Although, the model deviates from the off diagonal components of $\epsilon_{ij}$, the simplicity of the model and the qualitative accuracy of the model, makes it a popular choice.
4.4 Pressure Dependence of Models

The models discussed in the previous section have been evaluated at $Ma_c = 0.35$ and $Re_0 = 850$, with ambient pressures ranging from 1 atm to 100 atm. The model constants used in various models have been calibrated to fit the data obtained from the DNS. It has been observed that with increase in ambient pressure, the absolute magnitude of all the budget terms increase. However, the relative magnitude of various terms with respect to one another evaluated at a particular pressure remains unchanged.

4.4.1 Effects on Compressibility, Production and Dissipation Terms

The density fluctuation term ($\zeta_{ij}$) is observed to increase with pressure but still remains relatively smaller in magnitude compared to diffusion and pressure strain terms. The dissipation term ($\epsilon_{ij}$) has been observed to be of the same order of magnitude as the density fluctuation term. The effect of ambient pressures on compressibility and dissipation terms has been presented in Figs. 4.41-4.42. In most RSM based modeling studies, the effects of $\zeta_{ij}$ are neglected. However, the $\epsilon_{ij}$ term is modeled as it physically represents the effects of dissipation. In the high speed compressible mixing layer simulations by Vreman, Sandham and Luo [127], and Pantano and Sarkar [128], the focus has been on evaluation of effects of increasing Mach numbers on the Reynolds stress budget terms at ambient pressures of $P_0 = 1$ atm where $O(\zeta_{ij}) < O(\epsilon_{ij})$. The same cannot be said about the current study where $O(\zeta_{ij}) \approx O(\epsilon_{ij})$ especially at large ambient pressures. Thus, for a realistic reproduction of the Reynolds stresses at high ambient pressures, the density fluctuation term must be modeled.

In the aforementioned studies, the dissipation rates have been reported to remain unchanged with increasing Mach numbers while the absolute magnitudes of production have been reported to reduce with increasing Mach numbers. However, the rates of production and dissipation in the current study show an almost linear growth with increase in pressure. Unlike the models for diffusion and pressure-strain terms that show variation with pressure, the model for the dissipation term remains consistent with change in pressure. The dissipation rate ($\epsilon_{ij}$) in the budget equation is observed to be of the same order of magnitude as the isotropic dissipation rate tensor calculated from the DNS. This is due to the fact that the smallest scales of motion at which dissipation takes place can be considered isotropic. However, in RANS, solution of an additional transport equation
for $\epsilon$ is required. This transport equation in turn contains model constants that may vary with pressure. Thus, consistency of a model with pressure cannot be conclusively said until solution of an additional transport equation for $\epsilon$ is evaluated. The change of production with pressure is presented in Fig. 4.43.

### 4.4.2 Diffusion Models

In studies of mixing layers at high Mach numbers [127, 128], the magnitude of diffusion is observed to reduce in absolute value across the mixing layer and the turbulent diffusion is observed to be higher in magnitude than pressure diffusion. In a study of flow over airfoil at atmospheric pressures by Cecora *et al.* [129], the pressure diffusion is found to be negligible compared to viscous diffusion in the molecular diffusion term. However, in this study, the magnitude of the diffusion term is observed to increase non-linearly with pressure across the jet cross section as indicated in Fig. 4.44. Further, the absolute magnitude of molecular diffusion is observed to be much larger than that of turbulent diffusion. The major contributor to the molecular diffusion ($D_{ij}^m = D_{ij}^v + D_{ij}^p$) term is determined to be pressure diffusion:

\[
D_{ij}^p \gg D_{ij}^v,
D_{ij}^m \approx D_{ij}^p,
D_{ij}^p \gg D_{ij}^t,
D_{ij} \approx D_{ij}^p.
\]

The relative magnitudes of turbulent, viscous and pressure diffusion terms are presented in Figs. 4.45-4.52. The modeling approaches discussed in the Section (4.3.2) usually neglect the contribution from pressure diffusion when modeling molecular diffusion. In this work, the pressure diffusion term is observed to be 3 orders of magnitude higher than the viscous diffusion term at $P_0 = 1atm$. As a result, at atmospheric pressure the model constant ($C_m$) in Eq.(4.26) is determined to be approximately $10^3$ when compared to $C_m = 1$ in the base model. At larger pressures the viscous and pressure diffusion terms are observed to be of comparable magnitudes. As a result, the model constant $C_m$ is observed to reduce with increase in pressure. The model constants for turbulent diffusion are also observed to change with increase in pressure. The model constants for turbulent diffusion models are presented in Table (4.1).
To study the change of $C_t$ with pressure, the individual terms of the turbulent diffusion models ($\bar{p}, k^2/\epsilon, k/\epsilon, \partial R_{ij}/\partial x_k$) are calculated from the DNS. It is observed that the average density increases linearly with pressure, while the ratios of turbulent kinetic energy and dissipation rates remain invariant with change in pressure. The gradients of the Reynolds stresses in the models increase asymptotically with increase in pressure. This indicates intensification of turbulence (rate of production and diffusion) within shear flow with increase in pressure. However, this rate is observed to saturate at very large pressures [Figs. 4.53-4.61]. As a result, the model constants for turbulent diffusion reduces non-linearly with increase in pressure.

4.4.3 Pressure Strain Models

The magnitudes of the pressure strain tensor calculated from the DNS are observed to increase non-linearly with pressure. In the studies of evaluation of pressure strain models at various Mach number regimes by Gomez and Girimaji [126], it was observed that at low Mach number regimes ($Ma_c << 1$), the pressure strain correlation could be adequately modeled by an incompressible pressure strain model. A similar trend is observed in this study where the standard incompressible models (LRR, SSG) perform as well as the compressible model (GG). The calibrated model constant ($C_P$) in Eq.(4.38), that accounts for the effects of compressibility is small. However, with the standard model constants presented in Section (4.3.3.1), the models are 3 orders of magnitude smaller than the pressure strain obtained from DNS. The variation of model constants with pressure ($C_{new}$) are presented in Table (4.2). The factor ($n_H$) in the table represents a common multiplier for all the standard model constants ($C_{1 new} = n_H C_1, C_{2 new} = n_H C_2, C_{3 new} = n_H C_3, C_{4 new} = n_H C_4, C'_{1 new} = n_H C'_1, C'_{P new} = n_H C'_P$).

From the trend of $n_H$ it can be seen that the model constants for pressure strain models jump by a large factor with change in ambient pressure. An order of magnitude analysis of the terms in the model ($\bar{p}, k, \epsilon, b_{ij}, \bar{s}_{ij}, \Omega_{ij}$) is performed and the most significant contributor to the trend of the model is determined to be the rate of dissipation ($\epsilon$). The density, turbulent kinetic energy, strain and rotation tensors are observed to increase linearly, while the anisotropy tensor remains invariant with change in pressure. However, the dissipation rate is seen to increase by a factor of $\approx 10^3$ when the ambient pressure increases from 1atm to 35atm. This suggests that with increase in ambient pressure a major component of the shear energy is redistributed into the dissipation term by the pressure strain. The rates of dissipation along with production and diffusion become significantly
high with increasing pressure. At very large pressures the change of rate of dissipation is observed to reduce.

4.5 Conclusions

A common factor that affects the accuracy of all the models used in RSM is determined to be the modeling constants. The predictions of diffusion models with a single model constant are qualitatively similar to the DNS (predict similar mean rates of diffusion) but may not follow the trends exactly. This is also due to the fact that mathematically the diffusion process may be approximated by a second order derivative with a simple diffusion coefficient. However, the effects of the flow physics on the model constants must be taken into account before application of the model. From a rudimentary analysis in this study, it is observed that ambient pressure at a fixed Mach number and Reynolds number affects the model constants by a large factor. The ambient pressure causes the flow physics (convection, diffusion, dissipation, strain, rotation) to change which in turn affect the model constants. A similar observation can be made about the pressure strain model. Although the model depends upon a number of modeling constants unlike the diffusion models, the trends predicted are still only qualitatively similar to DNS. The physical process that dictates the pressure strain is complex and various components of the model are affected differently by the change in ambient pressure. These effects may become significantly different with change in Reynolds number at different Mach number regimes. Thus a careful consideration of the effects of flow physics on various modeling constants must be made before application of a model. In this work, the budget analysis and modeling of the Reynolds stress tensor alone has been presented. A similar approach may be applied towards modeling of turbulent mass flux \( \rho Y' u'_j \) and turbulent energy flux terms \( \rho e'_j u'_j \). However, the modeling constants chosen for the eddy diffusivity term \( \mu_t \) used in turbulent mass or energy flux models must be consistent with that of the Reynolds stress model. This would require optimization of the modeling constants that fit all the data (Reynolds stress, mass flux, energy flux).
Table 4.1: Variation of diffusion model constants with ambient pressure. LL model refers to Lien and Leschziner model. DH, MH and HL models refer to Daly and Harlow, Mellor and Herring and Hanjalic and Launder models, respectively.

<table>
<thead>
<tr>
<th>$P_0$(atm)</th>
<th>LL model</th>
<th>DH, MH, HL model</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$C_p$</td>
<td>$C_{m}$</td>
</tr>
<tr>
<td>1</td>
<td>20</td>
<td>1</td>
</tr>
<tr>
<td>10</td>
<td>0.21</td>
<td>1</td>
</tr>
<tr>
<td>35</td>
<td>0.007</td>
<td>1</td>
</tr>
<tr>
<td>70</td>
<td>0.002</td>
<td>1</td>
</tr>
<tr>
<td>100</td>
<td>0.001</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 4.2: Variation of pressure-strain model constants with ambient pressure. The multiplier ($n_\Pi$) indicates the factor that the standard model constants ($C_1, C_2, C_3, C_4, C_1', C_P$) of the baseline models are multiplied by to fit the pressure strain obtained from the DNS.

<table>
<thead>
<tr>
<th>$P_0$(atm)</th>
<th>Multiplier ($n_\Pi$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>LRR</td>
</tr>
<tr>
<td>1</td>
<td>800</td>
</tr>
<tr>
<td>10</td>
<td>100</td>
</tr>
<tr>
<td>35</td>
<td>20</td>
</tr>
<tr>
<td>70</td>
<td>8</td>
</tr>
<tr>
<td>100</td>
<td>3</td>
</tr>
</tbody>
</table>

Table 4.1: Variation of diffusion model constants with ambient pressure. LL model refers to Lien and Leschziner model. DH, MH and HL models refer to Daly and Harlow, Mellor and Herring and Hanjalic and Launder models, respectively.

Table 4.2: Variation of pressure-strain model constants with ambient pressure. The multiplier ($n_\Pi$) indicates the factor that the standard model constants ($C_1, C_2, C_3, C_4, C_1', C_P$) of the baseline models are multiplied by to fit the pressure strain obtained from the DNS.
Figure 4.1: Reynolds stress budget at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $\theta_0 = 1\text{ atm}$. 
Figure 4.2: Reynolds stress budget at $x = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 100$ atm.
Figure 4.3: Reynolds stress budget at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $M_{ac} = 0.35$, and $P_0 = 35$ atm.
Figure 4.4: Reynolds stress budget at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 700\text{ atm}$.
Figure 4.5: Reynolds stress budget at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_0 = 0.35$, and $P_0 = 100$ atm.
Figure 4.6: Balance of convection term and sum of diffusion, production, dissipation, pressure-strain and density-fluctuation terms at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 1atm$. 
Figure 4.7: Balance of convection term and sum of diffusion, production, dissipation, pressure-strain and density-fluctuation terms at $x_1 = 10D_{jet}$ at $Re_0 = 850$, $Ma_e = 0.35$, and $P_0 = 10$ atm.
Figure 4.8: Balance of convection term and sum of diffusion, production, dissipation, pressure-strain and density-fluctuation terms at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 35$ atm.
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Figure 4.10: Balance of convection term and sum of diffusion, production, dissipation, pressure-strain and density-fluctuation terms at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 100\text{atm}$.
Figure 4.11: Balance of $C_{ij}$ and $\beta_{ij} - \zeta_{ij}$ at $x_1 = 15D_{\text{jet}}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 1\text{ atm}$. 
Figure 4.12: Balance of $C_{ij}$ and $\beta_{ij} - \zeta_{ij}$ at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 10\text{ atm}$. 
Figure 4.13: Balance of $C_{ij}$ and $\beta_{ij} - \xi_{ij}$ at $x_1 = 15D_{jet}$ at $Re_0 = 850$, $Ma_c = 0.35$, and $P_0 = 35\text{ atm}$. 

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Figure 4.17: Diffusion term compared against Lien and Leschziner model at $P_0 = 10$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 

\[101 \times \left( \frac{\nu_t \partial^2 \theta}{\varepsilon \partial^2 \theta} \right) / \nu_t \partial \theta \]

\[101 \times \left( \frac{\nu_t \partial^2 \theta}{\varepsilon \partial^2 \theta} \right) / \nu_t \partial \theta \]

\[101 \times \left( \frac{\nu_t \partial^2 \theta}{\varepsilon \partial^2 \theta} \right) / \nu_t \partial \theta \]

\[101 \times \left( \frac{\nu_t \partial^2 \theta}{\varepsilon \partial^2 \theta} \right) / \nu_t \partial \theta \]
Figure 4.18: Diffusion term compared against Lien and Leschziner model at $P_0 = 35\text{ atm}$, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.19: Diffusion term compared against Lien and Leschziner model at $P_0 = 70$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.20: Diffusion term compared against Lien and Leschziner model at $P_0 = 100$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.21: Molecular diffusion model of Daly and Harlow, Mellor and Herring, and Hanjalic and Launder at $P_0 = 1$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.22: Molecular diffusion model of Daly and Harlow, Mellor and Herring and Hanjalic and Launder at $P_0 = 10$ atm, $Re_0 = 850$, and $Ma_{\infty} = 0.35$. 

\[ 101 \times \left( \frac{\nu D_{eff}}{t_{eff}} \right) / \tilde{u} \]
Molecular diffusion model of Daly and Harlow, Mellor and Herring, and Hanjalic and Launder at $P_0 = 35$ atm, $Re_0 = 850$, and $Ma_{c_v} = 0.35$. 

Figure 4.23:
Figure 4.24: Molecular diffusion model of Daly and Harlow, Mellor and Herring and Hanjalic and Launder at $P_0 = 70$ atm, $Re_0 = 850$, and $Ma_{ce} = 0.35$. 
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Figure 4.28: Triple velocity moment at $P_0 = 35\, atm$, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.29: Triple velocity moment at $P_0 = 70 \text{ atm}$, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.30: Triple velocity moment at $P_0 = 100$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.31: Pressure-strain models at $P_0 = 1$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.32: Pressure strain models at $P_0 = 100\text{atm}$, $Re_0 = 850$, and $Ma_c = 0.35$. 
Figure 4.33: Pressure strain models at $P_0 = 35$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 

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DSSG --- LRR

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Figure 4.34: Pressure strain models at $P_0 = 700\text{ atm}$, $Re_0 = 850$, and $Ma_{cr} = 0.35$. 
Figure 4.35: Pressure strain models at $P_0 = 100$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 

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**Figure Legend:**
- **DNS**: Direct Numerical Simulation
- **LRR**: Large Eddy Simulation - RANS
- **GL**: Gradient-Limiter RANS
- **SSS**: Slowly Stretched Shocklets
- **GG**: Gradient-Growth RANS

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Figure 4.36: Dissipation model at $P_0 = 1\text{ atm}$, $Re_0 = 850$, and $Ma_0 = 0.35$. 

101 $\times (\frac{\partial u}{\partial x})^2 / \nu_0$

101 $\times (\frac{\partial v}{\partial x})^2 / \nu_0$

101 $\times (\frac{\partial w}{\partial x})^2 / \nu_0$

101 $\times (\frac{\partial u}{\partial y})^2 / \nu_0$

101 $\times (\frac{\partial v}{\partial y})^2 / \nu_0$

101 $\times (\frac{\partial w}{\partial y})^2 / \nu_0$

101 $\times (\frac{\partial u}{\partial z})^2 / \nu_0$

101 $\times (\frac{\partial v}{\partial z})^2 / \nu_0$

101 $\times (\frac{\partial w}{\partial z})^2 / \nu_0$
Figure 4.37: Dissipation model at $P_0 = 10\,\text{atm}$, $Re_0 = 850$, and $Ma_c = 0.35$. 

\[ t_0 \times \left( \frac{\nu_0}{\nu_0^\prime} \right) / \Delta \]
Figure 4.38: Dissipation model at $P_0 = 35$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 

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Figure 4.39: Dissipation model at $P_0 = 70$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 

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[Graphs showing dissipation model comparisons]
Figure 4.40: Dissipation model at $P_0 = 100$ atm, $Re_0 = 850$, and $Ma_c = 0.35$. 
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Figure 4.55: Variation of turbulent dissipation rate with pressure.
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Figure 4.60: Variation of rotation tensor with pressure.

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Bibliography


[18] A. Uzun. 3-D Large Eddy Simulation for jet aeroacoustics. PhD dissertation, Purdue University, Department of Mechanical Engineering, December 2003.


